Научном већу Института за физику у Београду

Предмет: Молба за покретање поступка за избор у звање виши научни сарадник

Молим Научно веће Института за физику у Београду да, у складу са Правилником о стицању истраживачких и научних звања Министарства науке, технолошког развоја и иновација Републике Србије, покрене поступак за мој избор у звање виши научни сарадник.

У прилогу достављам:

1. Мишљење руководиоца лабораторије са предлогом чланова комисије;

2. Попуњен Образац за материјал за покретање поступка избора у научно звање (подаци о кандидату, преглед научне активности, приказ најзначајнијих резултата, показатељи успеха у научноистраживачком раду, библиографија кандидата, квантификација научних резултата);

3. Додатне прилоге (копију решења о претходном избору у звање, доказе о руковођењу пројектима, доказе о рецензирању, доказе о предавањима по позиву, доказе о публикацијама категорије М34, податке о цитираности, доказе о наградама и признањима, стечене сертификате у оцењиваном периоду, доказе о менторствима, доказе о улози гостујућег уредника часописа и доказе о запослењима у иностраним научноистраживачким институцијама).

У Београду,
19. марта 2026. године

С поштовањем,

др Миљан Дашић
научни сарадник

УНИВЕРЗИТЕТ У БЕОГРАДУ
ИНСТИТУТ ЗА ФИЗИКУ | БЕОГРАД
ИНСТИТУТ ОД НАЦИОНАЛНОГ ЗНАЧАЈА ЗА РЕПУБЛИКУ СРБИЈУ
Прегревица 118, 11080 Земун - Београд, Република Србија
Телефон: +381 11 3713000, Факс: +381 11 3162190, www.ipb.ac.rs
ПИБ: 100105980, Матични број: 07018029, Текући рачун: 205-66984-23

Научном већу Института за физику у Београду

Предмет: Мишљење руководиоца о избору др Миљана Дашића у звање виши научни сарадник

Др Миљан Дашић је запослен у Лабораторији за примену рачунара у науци у оквиру Центра за изучавање комплексних система Института за физику у Београду. У свом истраживачком раду бави се темама везаним за моделирање нанотриболошких феномена у различитим системима и материјалима.

С обзиром да др Миљан Дашић испуњава све услове прописане Правилником о стицању истраживачких и научних звања и Законом о науци и истраживањима, сагласна сам са покретањем поступка за избор др Миљана Дашића у звање виши научни сарадник.

Предлажем следећи састав комисије за избор др Миљана Дашића у звање виши научни сарадник:

1. др Игор Франовић, научни саветник, Институт за физику у Београду,
2. др Игор Станковић, научни саветник, Институт за физику у Београду,
3. проф. др Сунчица Елезовић-Хаџић, редовни професор, Физички факултет, Универзитет у Београду

Марија Митровић Данкулов

др Марија Митровић Данкулов,
научни саветник
руководилац Лабораторије за примену рачунара у науци

Материјал уз захтев за избор др Миљана Дашића у звање виши научни сарадник

1. ПОДАЦИ О КАНДИДАТУ

Име и презиме: Миљан Дашић
Година рођења: 1990
Радни статус: запослен
Назив институције у којој је запослен/а: Институт за физику у Београду
Претходна запослења: /

Образовање
Основне академске студије: 2009-2013, Електротехнички факултет, Универзитет у Београду
Одбрањен мастер рад: 2014, Електротехнички факултет, Универзитет у Београду
Одбрањена докторска дисертација: 2019, Физички факултет, Универзитет у Београду

Постојеће научно звање: научни сарадник
Научно звање које се тражи: виши научни сарадник

Датуми избора у стечена научна звања (укључујући и постојеће)
научни сарадник: 27.3.2020. (реизбор 22.11.2024.)
виши научни сарадник: /

Област науке у којој се тражи звање: природно-математичке науке
Грана науке у којој се тражи звање: физика
Научна дисциплина у којој се тражи звање: Физика кондензоване материје и физика материјала
Назив матичног научног одбора којем се захтев упућује: МНО за физику

Стручна биографија

Миљан Дашић рођен је 3.11.1990. године у Параћину, где је завршио основну школу и природно-математички смер гимназије. Основне академске студије на Одсеку за физичку електронику Електротехничког факултета Универзитета у Београду завршио је у јулу 2013. године, са просечном оценом 9.93. Мастер академске студије на истом одсеку и факултету завршио је у јулу 2014. године, са просечном оценом 10.00. Свој мастер рад урадио је у Лабораторији за примену рачунара у науци на Институту за физику у Београду, под менторством др Игора Станковића. Октобра 2014. године уписао је докторске академске студије на Физичком факултету Универзитета у Београду, на смеру физика кондензоване материје и статистичка физика. Докторске студије на Физичком факултету завршио је са просечном оценом 9.75. Вредно је поменути да је полагао и два диференцијална испита са основних академских студија физике (Теоријска Механика и Теорија Кондензованог Стања), и на оба је добио оцену 10. Дана 23. септембра 2019. године, одбранио је своју докторску дисертацију „Modeling the Behaviour of Confined Dipolar and Ionic Systems" на Физичком факултету Универзитета у Београду, која је урађена под менторством др Игора Станковића. Од новембра 2014. године запослен је на Институту за физику у Београду у Лабораторији за примену рачунара у науци, у оквиру Националног центра изузетних вредности за изучавање комплексних система, где је до децембра 2019. године био ангажован на пројекту основних истраживања „Моделирање и нумеричке симулације сложених вишечестичних система" (ОН171017), којим је руководио др Антун Балаж, а од јануара 2020. године је ангажован институционално. У звање истраживач сарадник изабран је у априлу 2017. године, а у звање научни сарадник у марту 2020. године. У периоду од 1.11.2019. године до 31.12.2021. године радио је на Чешком техничком универзитету у Прагу у Чешкој као постдокторски истраживач. По завршетку наведеног постдока, вратио се у Београд и провео је 2022. годину радећи на свом матичном Институту за физику у Београду. Схватајући значај међународних сарадњи у модерној науци, а нарочито постдокторских усавршавања у иностранству, потражио је нови постдок. На основу позитивних утисака са првог постдока и високог нивоа знања чешког језика, радо је прихватио могућност повратка у Праг. Од 1.3.2023. године до 31.12.2024. године радио је на Институту за органску хемију и биохемију Чешке академије наука у Прагу као постдокторски истраживач. Свој научни ангажман у

Прагу наставио је у јануару 2025. године на Институту за физичку хемију Јарослав Хејровски Чешке академије наука. Учествовао је у више националних, билатералних и међународних пројеката. Добитник је студентске награде Института за физику у Београду за најбољу докторску дисертацију одбрањену током 2019. године и награде Привредне коморе Србије за најбоље докторске дисертације са применама у привреди за академску школску годину 2018/2019. Као члан COST акције CA21121 MecaNano, добио је грант за учешће на међународној конференцији "The 11th International Conference on Multiscale Materials Modeling (mmm11)" која се одржала у септембру 2024. године у Прагу.

2. ПРЕГЛЕД НАУЧНЕ АКТИВНОСТИ

Научноистраживачки рад кандидата припада научној дисциплини физика кондензоване материје и физика материјала, а заснива се на теорији, аналитичким методима и рачунарским симулацијама. Његова научна активност у оцењиваном периоду може се поделити на три истраживачка правца:

2.1 Моделовање и симулације различитих нанотриболошких система

Нанотрибологија се бави физичким феноменима трења, хабања и подмазивања на наноскали, при чему тема истраживања могу бити различити материјали. У оквиру датог истраживачког правца, кандидат је помоћу моделовања и симулација изучавао три нанотриболошка система: аморфне ванадијум-оксиде, мешавине фосфонијумсих јонских течности са водом и молибденијум-дисулфид. Заједнички циљ свих поменутих истраживања је одређивање структуре материјала при одређеним термодинамичким и механичким условима (температура, притисак, механичке деформације попут примењене нормалне силе или смицања), а потом и одређивање триболошких карактеристика (механизам и тип трења, коефицијент трења, хабање, ефекат подмазивања). Наведени научни приступ омогућава добијање структура-особине (structure-properties) релације, која даје драгоцени увид у потенцијалне технолошке примене испитиваних триболошких система. Такође, резултати постигнути у овим истраживањима омогућују симулациону референцу и информишу паралелна (кроз синергију симулације-експерименти) или будућа експериментална истраживања над истим триболошким системима.

2.2 Развој и примене метода нормалне динамике

Метод молекуларне динамике (Molecular Dynamics – MD) је један од најраширенијих и најстандарднијих метода моделовања у физици кондензоване материје и физици материјала. То међутим не спречава развој алтернативних метода моделовања, који у конкретним проблемима могу показати бољу применљивост и/или рачунарске перформансе од молекуларне динамике. Кандидат је конкретно радио на развоју и верификацији иновативног метода у физици материјала, названог нормална динамика (Normal Dynamics – ND), зато што представља еквивалент MD-а у реципрочном простору. Употреба нормалних координата је и одредница која је дала назив овом новом методу. MD се у суштини своди на решавање Њутнових једначина кретања датог система атома у картезијанским координатама. Нормална динамика преиначава Њутнове једначине кретања помоћу фононских нормалних мода, користећи адекватно узорковање реципрочног простора, што омогућава: повећање рачунарске ефикасности (тј. скраћивање времена извршавања рачунарских програма) бирањем који и колико таласних вектора Бриуленове зоне ће бити разматрани, као и узимање у обзир дисторзија преко великих атомских растојања, без потребе за коришћењем великих симулационих кутија.

2.3 Моделовање и симулације хидратисаних Нафион мембрана

Горивне ћелије са мембраном за размену протона (Proton Exchange Membrane Fuel Cells – PEMFC), које користе водоник као гориво, представљају перспективно решење за широк спектар примена конверзије енергије, при чему је Нафион најчешће коришћени материјал за

израду мембрана. Количина воде коју апсорбује Нафион мембрана има кључни утицај на механичке особине и операбилност мембране, зато што ниво хидратације одређује транспортна својства мембране. Потребно је одредити оптималну хидратацију која омогућава ефикасан транспорт протона, али не нарушава механичку стабилност мембране. У оквиру датог истраживачког правца, остварена је сарадња са колегама из немачке корпорације Фројденберг, који су експериментално одредили зависност густине мембране од нивоа хидратације. Кандидат је био укључен у симулациони аспект поменуте сарадње. Резултати добијени симулацијама молекуларне динамике омогућили су повезивање експерименталних резултата са молекуларним опажањима. Разумевање начина на који мембрана реагује на промене садржаја воде омогућава пренос механизама са молекуларног нивоа до нивоа примене у индустријским PEMFC системима.

3. ПРИКАЗ НАЈЗНАЧАЈНИЈИХ РЕЗУЛТАТА

3.1 Триболошке карактеристике ванадијум оксида (рад [1])

У оквиру дате теме, кандидат је радио на развоју и применама симулација молекуларне динамике на нанотриболошки систем који се састоји од два кристална слоја направљена од ванадијум-пентоксида (V_2O_5) и пет различитих стохиометрија аморфног ванадијум-оксида смештених између датих кристалних слојева. Циљ је био испитати нанотриболошке карактеристике аморфних ванадијум-оксида при различитим температурама и примењеној нормалној сили на горњи кристални V_2O_5 слој. Ради симулирања динамичког формирања и прекидања ковалентних веза између атома ванадијума и кисеоника, чиме се постиже реалистично моделовање, примењиван је метод реактивне молекуларне динамике, који представља подтип општег метода молекуларне динамике. Конкретно, симулирано је следећих пет стохиометрија ванадијум-оксида: {V_2O_3, V_3O_5, V_8O_{15}, V_9O_{17}, VO_2} које су одабране на основу постојећих експерименталних истраживања и своје релевантности у технолошким применама. Занимале су нас триболошке перформансе испитиваних ванадијум-оксида при условима повишене температуре и притиска, тако да смо применили температуру од {600, 800, 1000} [K] и притисак од {1, 2, 3, 4} [GPa], укључујући и референтни случај без примењеног спољног притиска. Све разматране стохиометрије омогућавају подмазивање са релативно ниским коефицијентом трења од 0.2, што је драгоцена информација која је релевантна за дизајн премаза (coating) у којима је ванадијум у улози подмазивачког агента. Општа тенденција смањивања коефицијента трења са порастом температуре представља триболошки ефекат који је користан за прилагодљиво подмазивање. Примећен је растући тренд отклона силе трења (што је повезано са ефектом адхезије), са смањењем садржаја кисеоника у ванадијум-оксидима. Резултати рада на овој теми представљени су у научном раду "Tribological properties of vanadium oxides investigated with reactive molecular dynamics" који је објављен 2022. године у водећем међународном часопису категорије M21a+ Tribology International. Кандидат је дао веома значајан допринос изради овог рада, тако да је у улози водећег аутора, као и кореспондинг аутора.

3.2 Утицај садржаја воде на транспортне и термодинамичке особине фосфонијумских јонских течности (рад [5])

У оквиру рада на датој теми, одређене су транспортне и термодинамичке карактеристике фосфонијумских јонских течности помешаних са водом, у различитим односима. Кроз детаљну студију засновану на симулацијама молекуларне динамике, добијени су ефекти садржаја воде у поменутим мешавинама на температуру кључања, дифузију и вискозност. Тиме су остварени драгоцени увиди на молекуларном нивоу у утицај количине воде на карактеристике јонских течности помешаних са водом. Дати системи, поред фундаменталног значаја, поседују и значај са аспекта технолошких примена. Наиме, фосфонијумске јонске течности имају потенцијал као еколошка мазива, при чему се издвајају својим једноставним процесом синтезе. Са високом вискозношћу, високом термалном стабилношћу и малим

притиском паре, јонске течности показују свестрану природу која их истиче као оптималан избор у захтевним и неприступачним оперативним срединама. Резултати добијени у оквиру ове теме представљени су у научном раду "Effects of Water Content on the Transport and Thermodynamic Properties of Phosphonium Ionic Liquids" који је објављен 2024. године у међународном часопису категорије M22 Langmuir, на коме је кандидат други аутор. Кандидатов допринос је превасходно везан за развој скрипти симулација молекуларне динамике, као и за ревизију и едитовање рада.

3.3 Улога заробљених молекула воде у триболошким контактима са трењем на резолуцији кристалне решетке материјала (рад [3])

Улога молекула воде који су заробљени у триболошком наноконтакту који се експериментално испитује помоћу микроскопа на бази атомских сила (Atomic Force Microscope – AFM) била је недовољно истражена и нејасна. У циљу изучавања и решавања поменутог научног проблема, кандидат је остварио сарадњу са експерименталним тимом проф. Ронена Берковича са Бен Гурион Универзитета из Израела. Систем који је експериментално и симулационо истраживан састоји се од пробе (probe) састављене од аморфног силицијум-диоксида (SiO_2) и једнослојног кристала молибденијум-дисулфида (MoS_2) као узорка (sample), при чему су у наноконтакту присутни молекули воде.
У експериментима постоје две количине и просторне расподеле молекула воде: кондензована водена капилара услед одређене влажности ваздуха, као и AFM проба наменски потпуно потопљена у воду. У симулацијама су имплементирана поменута два система, уз још један додатни који је имао улогу референтног система: проба обложена водом (water coated probe), при чему је количина воде недовољна да би се формирала капилара. Суштински, испитиван је утицај количине и просторне расподеле молекула воде на наноскопско трење, у клизећем контакту пробе и узорка. Резултати, како експеримената тако и симулација, показују да се stick-slip трење (тип трења који се јавља при клизању преко кристалних површина) на резолуцији константе решетке узорка може постићи са заробљеним молекулима воде присутним у наноконтакту, при широком опсегу интензитета нормалне силе примењене на пробу. Резултати рада на овој теми представљени су у научном раду "Role of Trapped Molecules at Sliding Contacts in Lattice-Resolved Friction" који је објављен 2024. године у водећем међународном часопису категорије M21a ACS Applied Materials & Interfaces. Кандидат је дао веома значајан допринос изради овог рада, тако да је у улози водећег аутора, као и кореспондинг аутора. Препознавањем синергије експертиза из домена симулација и експеримената, као и иницирањем сарадње српске и израелске научноистраживачке институције, кандидат је дао позитиван пример остваривања међународне научне сарадње.

3.4 Развој, софтверска имплементација и примене метода нормалне динамике (рад [4])

Теоријска разматрања метода нормалне динамике наговестила су његове предности над опште прихваћеним и примењиваним методом молекуларне динамике, приликом примена у специфичним проблемима. Дати приступ је аналитички изведен и имплементиран у Фортран код, који је потом примењен у три студије случаја. Главни циљ је био верификација развијеног метода и софтвера, али и указивање могућности и значаја његове употребе. У првој студији случаја приказана је општа стратегија узорковања реципрочног простора, а конкретно је рачуната фононска дисперзија кристалног силицијума; у другој студији случаја приказана је применљивост метода у изучавању стабилизационог ефекта температуре у α-уранијуму; у трећој студији случаја истраживана је карактеризација Раманског спектра на различитим температурама у MoS_2/MX_2 хетероструктурама на бази дихалкогенида прелазних метала. На тако разноликим студијама случаја, приказано је и дискутовано о томе како метод нормалне динамике поседује општи значај, и може се применити на симулирање периодичних[а], семипериодичних[б] и коначних[в] система, попут кристала[а], плоча (slabs)[б] и молекула[в], респективно. Изворни код (source code) комплетног Фортран софтвера, који је кандидат у сарадњи са двојицом колега развио, налази се на линку: https://github.com/acammarat/pindol. На

датом линку се налазе и помоћни софтвери који се користе за прет- и пост- процесирање симулација нормалне динамике, као и примери примене са детаљним упутствима за нове кориснике. Резултати рада на овој теми представљени су у научном раду "Integrating Newton's Equations of Motion in the Reciprocal Space" који је објављен 2024. године у водећем међународном часопису категорије M21 Journal of Chemical Physics на коме је кандидат други аутор. Кандидатов допринос се односи на теоријски развој метода и његову софтверску имплементацију, потом на рад на истраживању и формалној анализи, као и на ревизију и едитовање рада.

3.5 Повезивање густине и наноскалне кристалиничности са хидратацијом у Нафион мембранама (рад [2])

Фокус истраживања у оквиру ове теме био је на Нафион 117 протон-размењивачкој мембрани и на питању како се промена хидратације (λ = број молекула воде по сулфонатној групи) одражава на густину, кристалиничност и наноскалну морфологију водене фазе. Остварена је сарадња са колегама из немачке корпорације Фрojденберг, који су се бавили експерименталним делом рада на овој теми. Наиме, синергијским приступом смо комбиновали експериментална мерења густине (хидростатичко мерење по Архимедовом принципу) са симулацијама молекуларне динамике у више режима морфологије: аморфно, полукристално и кристално стање (различите термомеханичке историје, укључујући смицање ради убрзавања структурног уређења). На нивоу симулација примењују се полидисперзна Вороној теселација и анализа слободне запремине (Fractional Free Volume – FFV), као и DBSCAN (Density-Based Spatial Clustering of Applications with Noise) кластеровање молекула воде, чиме се раздваја ефективна густина Нафиона и конфиниране воде у каналима/кластерима. Кључни налаз је изражена корелација између кристалиничности и ефективне густине Нафион фазе: веће уређење подразумева компактније паковање и вишу густину, уз ефекат сатурације при високој кристалиничности. Истовремено, вода показује јасан прелаз од изолованих молекула/кластера при ниској хидратацији ка перколационим мрежама при вишој хидратацији, нарочито у уређенијим (кристалним) конфигурацијама, где се формирају израженији повезани канали. Посебно је значајна чињеница да густина конфиниране воде може достићи вредности до приближно 1.2 g/cm^3, што указује на наноскални "compression/ordering" ефекат у ограниченим доменима, различит од балк воде. Предложили смо и квантитативни (феноменолошки) модел који повезује унос воде и промене ефективне густине, чиме смо дали предиктивни оквир за оптимизацију хидратације, транспорта и механичке стабилности мембрана у реалистичним условима. Резултати рада на овој теми презентовани су у научном раду "Linking Density and Nanoscale Crystallinity to Hydration in Nafion PEMFC Membranes: Insights from Experiment and Molecular Dynamics Simulations" који је објављен 2026. године у водећем међународном часопису категорије M21a Small Structures на коме је кандидат претпоследњи аутор. Кандидатов допринос припада домену симулација молекуларне динамике, као и ревизији и едитовању рада. У реализацији рада на овој теми, кандидат је био у улози ментора млађег сарадника (докторанда) Матеје Јовановића, који је у улози водећег аутора овог рада.

4. ПОКАЗАТЕЉИ УСПЕХА У НАУЧНОИСТРАЖИВАЧКОМ РАДУ

4.1. Утицајност

Према Scopus бази података, научни радови кандидата цитирани су укупно 123 пута, при чему је вредност Хиршовог индекса 8. Изузимајући аутоцитате, број цитата је 111, а Хиршов индекс је 7. У прилогу 6 је дат извештај из Scopus базе генерисан на дан 18.3.2026. године.

4.2. Међународна научна сарадња

Кандидат је остварио међународну научну сарадњу кроз усавршавање на иностраним научноистраживачким институцијама:

(1) постдокторско усавршавање на Чешком техничком универзитету у Прагу (у периоду 1.11.2019 – 31.12.2021)

(2) постдокторско усавршавање на Институту за органску хемију и биохемију Чешке академије наука у Прагу (у периоду 1.3.2023 – 31.12.2024)

(3) постдокторско усавршавање на Институту за физичку хемију Јарослав Хејровски Чешке академије наука у Прагу (у току, започето 13.1.2025. године)

Докази о запослењу у наведеним иностраним научноистраживачким институцијама дати су у прилогу 11.

4.3. Руковођење пројектима и потпројектима (радним пакетима)

Кандидат је руководио на два радна пакета у оквиру пројекта "Scoring of Protein-Ligand Binding Affinity Predictions" на коме је радио током постдокторског усавршавања на Институту за органску хемију и биохемију Чешке академије наука у Прагу (2023 – 2024). Називи радних пакета на којима је кандидат руководио су:

(1) Развој и примене софтвера за аутоматизовану припрему протеинских структура за квантно-механички скоринг

(2) Развој и примене софтвера за селекцију структурних молекула воде који појачавају предикције афинитета везивања лиганда за протеин

Дати пројекат финансирао је наведени Институт, а радило се о интерном пројекту комерцијализације. У прилогу 2 је дат доказ о овом руковођењу, са информацијама о радним пакетима и улози кандидата у њиховој реализацији.

4.4. Уређивање научних публикација

Кандидат је у улози гостујућег уредника (Guest Editor) специјалног издања научног часописа Symmetry под називом "Symmetry/Asymmetry in Condensed Matter Physics and Engineering Applications". Према Кобсон бази категорија часописа Symmetry је M21; IF2 2024: 2.2; IF5 2024: 2.1. Докази о томе дати су у прилогу 10.
Напомена: важно је нагласити да наведено специјално издање до сада нема објављених радова, што значи да је улога гостујућег уредника формално испуњена, али како би била и суштински испуњена, треба сачекати објављивање радова. Релевантна информација је да је актуелни рок за слање радова 31.5.2026., са тиме што ће вероватно бити померен, што је уобичајена пракса у специјалним издањима научних часописа датог издавача.

4.5. Предавања по позиву (осим на конференцијама)

Кандидат је одржао два предавања по позиву у домаћим и иностраним институцијама у области науке и високог образовања (осим на конференцијама):

(1) предавање по позиву на манифестацији "Дани Фотонике" у децембру 2023. године на Електротехничком факултету Универзитета у Београду

(2) предавање по позиву на тренинг школи BLESSED пројекта Европске мреже доктората у новембру 2024. године на Универзитету Пикардије Жил Верн у Амјену у Француској

Докази о наведеним предавањима по позиву (осим на конференцијама) дати су у прилогу 4.

Поред два наведена предавања по позиву (осим на конференцијама), може се истаћи да је кандидат учествовао у организацији две међународне научне радионице, на којима је и одржао предавања:

(1) међународна научна радионица "Argentinian-Serbian Nanotechnology Workshop: Challenges in bridging theory and experiments" одржана у новембру 2024. године на Институту за физику у Београду

(2) међународна научна радионица "Workshop on Integrating Simulations and Experiments for Advanced Applications" одржана у јануару 2026. године у Српској академији наука и уметности у Београду

Докази о организацији и предавањима на наведеним радионицама дати су у прилогу 4.

Што се тиче предавања по позиву на конференцијама (резултати категорије М32), у прилогу 4 су дати докази да су у питању међународне конференције, на основу чињенице да имају научни комитет са члановима из бар 5 различитих земаља.

4.6. Рецензирање пројеката и научних резултата

Кандидат је рецензирао 47 научних радова у часописима разних категорија: М21a+ (Tribology International), М21 (Polymers, Materials, Symmetry, …) и М22 (већи број часописа). Укупан број различитих часописа је 19, а укупан број различитих издавача је 4 (Springer Nature[1], Elsevier[2], Multidisciplinary Digital Publishing Institute (MDPI)[3], Frontiers[4]). Докази о рецензентским активностима кандидата дати су у прилогу 3.

4.7. Образовање научних кадрова

Кандидат је био ментор и члан комисије за одбрану мастер рада студента Матеје Јовановића под називом "Симулације структурних, термодинамичких и механичких карактеристика мешавине јонске течности и воде методом молекуларне динамике: пример $[bmim]^+[PF6]^-$ јонске течности", који је одбрањен на Физичком факултету Универзитета у Београду у септембру 2023. године.

Кандидат је био ментор на два пројекта на Семинару физике у Истраживачкој станици Петница која су успешно завршена презентацијом полазника на годишњој петничкој конференцији "Корак у науку" и објављивањем радова у "Петничким свескама".
Менторисаних петнички радови:

(1) "Испитивање течно-чврстог контакта ТМ јонских течности и кристалне подлоге методом молекуларне динамике"
година: 2019
полазници: Александар Филиповић и Матеј Вучковић

(2) "Анализа магнетних тубуларних структура у вертикалном хомогеном магнетном пољу"
година: 2022
полазник: Михајло Срећковић

Докази о наведеним менторствима дати су у прилогу 9.

Поред тога, кандидат је ментор на докторским академским студијама Матеје Јовановића, који је докторски студент на Физичком факултету Универзитета у Београду. Одбрана теме докторске дисертације очекује се у току 2026. године. Додатно, кандидат је ко-ментор (у оквиру свог ангажмана на Институту за физичку хемију Чешке академије наука у Прагу) на

докторским академским студијама Ашвати Пуламане, која је докторски студент на Математичко-физичком факултету Карловог Универзитета у Прагу. Израда њене докторске дисертације је у почетној фази, с обзиром да је колегиница тренутно на другој години докторских студија.

4.8. Награде и признања

Кандидат је добитник студентске награде Института за физику у Београду за најбољу докторску дисертацију одбрањену током 2019. године. Такође, добитник је награде Привредне Коморе Србије за најбоље докторске дисертације са применама у привреди за академску школску годину 2018/2019. Докази о поменутим наградама дати су у прилогу 7.

4.9. Допринос развоју одговарајућег научног правца

У складу са дефиницијом овог квалитативног услова, може се навести следеће: кандидат је објавио рад категорије М21а+ у часопису Tribology International (2022) на коме је водећи и кореспондинг аутор. Истраживања презентована у овом раду реализована су током постдока на Чешком техничком универзитету у Прагу, према томе немају везе са истраживањима из докторске дисертације. На датом раду нема коауторства са ментором са доктората. Наведени научни резултат представља допринос кандидата развоју научног правца рачунарске нанотрибологије.

Поред тога, у току је припрема рада који је у вези са истраживањима реализованим током кандидатовог постдока на Институту за органску хемију и биохемију Чешке академије наука у Прагу, на коме је водећи аутор. Додатно, очекује се објављивање радова у оквиру ангажмана на Институту за физичку хемију Чешке академије наука у Прагу који је у току, такође у својству водећег аутора. Дати радови ће представљати кандидатов допринос развоју научног правца рачунарске биофизике.

5. БИБЛИОГРАФИЈА КАНДИДАТА

Кандидат је до сада објавио укупно 10 радова у међународним научним часописима. У оцењиваном периоду има 5 објављених радова.

Радови у водећим међународним часописима (категорија М21а+) - оцењивани период:

[1] **M. Dašić**, I. Ponomarev, T. Polcar, and P. Nicolini,
"Tribological Properties of Vanadium Oxides Investigated with Reactive Molecular Dynamics",
Tribology International 175, 107795 (2022).
doi: 10.1016/j.triboint.2022.107795

Радови у водећим међународним часописима (категорија М21а) - оцењивани период:

[2] M. Jovanović, N. Bernhard, M. Baldofski, M. Rybicki, **M. Dašić**, and I. Stanković,
"Linking Density and Nanoscale Crystallinity to Hydration in Nafion PEMFC Membranes: Insights From Experiment and Molecular Dynamics Simulations",
Small Structures 7 (3), e202500573 (2026).
doi: 10.1002/sstr.202500573

[3] **M. Dašić**, R. Almog, L. Agmon, S. Yehezkel, T. Halfin, J. Jopp, A. Ya'akobovitz, R. Berkovich, and I. Stanković, "Role of Trapped Molecules at Sliding Contacts in Lattice-Resolved Friction",
ACS Applied Materials & Interfaces 16, 44249 (2024).
doi: 10.1021/acsami.4c08226

Радови у водећим међународним часописима (категорија М21) - оцењивани период:

[4] A. Cammarata, **M. Dašić**, and P. Nicolini,
"Integrating Newton's Equations of Motion in the Reciprocal Space",
Journal of Chemical Physics 161, 084111 (2024).
doi: 10.1063/5.0224108

Радови у међународним часописима (категорија М22) - оцењивани период:

[5] I. Stanković, **M. Dašić**, M. Jovanović, and A. Martini,
"Effects of Water Content on the Transport and Thermodynamic Properties of Phosphonium Ionic Liquids",
Langmuir 40, 9049 (2024).
doi: 10.1021/acs.langmuir.4c00372

Предавања по позиву са међународног скупа штампана у изводу (категорија М32) - оцењивани период:

[6] **M. Dašić**, A. Cammarata, and P. Nicolini,
"Phonon-Inspired Normal Dynamics of Lattices",
The 1st Virtual meeting WG2 of COST action CA21101 COSY, 6th February 2024,
Belgrade, Serbia, Book of Abstracts, page 25 (2024)

[7] **M. Dašić**,
"Computer-Aided Drug Design",
The Training School of COST action CA21101 COSY, 19-22 September 2023,
Belgrade, Serbia, Book of Abstracts, page 23-24 (2023)

Саопштења са међународног скупа штампана у изводу (категорија М34) – оцењивани период:

[8] M. Jovanović, M. Baldofski, N. Bernhard, M. Rybicki, **M. Dašić**, and I. Stanković,
"Mechanical Behavior of Nafion Membranes",
German Physical Society (DPG) Spring Meeting 2026, 8-13 March 2026,
Dresden, Germany (2026).

[9] **M. Dašić**, A. Poolamanna, M. Hazrati, and Š. Timr,
"Multi-Scale Computational Framework for Modeling Metabolic Pathways",
German Physical Society (DPG) Spring Meeting 2026, 8-13 March 2026,
Dresden, Germany (2026).

[10] **M. Dašić**, I. Stanković, M. Jovanović, A. Martini,
"Impact of Water Content on the Mechanical and Thermodynamic Properties of Phosphonium Ionic Liquids",
26th IUPAP Conference of Computational Physics (online), 3-7 November 2025

[11] M. Jovanović, N. Bernhard, M. Baldofski, M. Rybicki, **M. Dašić**, and I. Stanković,
"Correlation Between Nanoscale Crystallinity, Density, and Hydration in Nafion Membranes: Experimental and Molecular Dynamics Insights",
26th IUPAP Conference of Computational Physics (online), 3-7 November 2025

[12] S. J. Rodriguez, M. Jovanović, **M. Dašić**, I. Stanković,
"Comparisons of Interactions and Morphology During Aluminium Fluoride and Water Intercalation in Graphite",

The 13th Conference of the Serbian ceramic society "Advanced ceramis and application", 8-10 September 2025,
Belgrade, Serbia (2025)

[13] **M. Dašić**, A. Poolamanna, M. Hazrati, and Š. Timr,
"Multi-Scale Modeling of Enzyme-Substrate Interactions in Crowded Environments",
15th European Biophysics Congress, 30 June - 4 July 2025,
Rome, Italy (2025).

[14] A. Poolamanna, **M. Dašić**, M. Hazrati, and Š. Timr,
"Substrate Binding in Enzyme Clusters: Effects of Crowders and Transient Interactions",
15th European Biophysics Congress, 30 June - 4 July 2025, Rome, Italy (2025).

[15] **M. Dašić**, J. Fanfrlík, and J. Řezáč,
"Selecting Protein Crystal Structure for Optimal Scoring of Protein-Ligand Interactions",
MecaNano 3rd General Meeting, 19-21 May 2025,
Krakow, Poland (2025).

[16] **M. Dašić**, and I. Stanković,
"Role of Trapped Water Molecules at Sliding Contacts in Lattice-Resolved Friction Investigated with Molecular Dynamics", German Physical Society (DPG) Spring Meeting 2025, 16-21 March 2025,
Regensburg, Germany (2025).

[17] M. Jovanović, M. Baldofski, I. Stanković, M. Rybicki, and **M. Dašić**,
"Evaluating the Properties of Nafion PEMFC Membrane via MD Simulations",
German Physical Society (DPG) Spring Meeting 2025, 16-21 March 2025,
Regensburg, Germany (2025).

[18] **M. Dašić**, A. Cammarata, and P. Nicolini,
"Integrating Newton's Equations of Motion in the Reciprocal Space as a Novel Materials Modeling Technique",
11th International Conference on Multiscale Materials Modeling, 22-27 September 2024,
Prague, Czech Republic (2024).

[19] **M. Dašić**, and I. Ponomarev,
"Reactive Molecular Dynamics Study of the Nanotribological Properties of Oxidized Vanadium",
11th International Conference on Multiscale Materials Modeling, 22-27 September 2024,
Prague, Czech Republic (2024).

[20] I. Stanković, **M. Dašić**, M. Jovanović, and Ashlie Martini
"Effects of Water Content on the Transport and Thermodynamic Properties of Phosphonium Ionic Liquids",
The 12th Liquid Matter Conference – Liquids 2024, 22-27 September 2024,
Mainz, Germany (2024).

[21] **M. Dašić**, J. Fanfrlík, and J. Řezáč,
"Sensitivity of the Scoring of Protein-Ligand Binding Affinity Predictions on Protein Crystal's Geometry",
3rd International Conference on Noncovalent Interactions (ICNI2024), 17-21 June 2024,
Belgrade, Serbia (2024).

[22] **M. Dašić**, A. Cammarata, and P. Nicolini,
"Normal Dynamics - method development and applications",
MecaNano 2nd General Meeting, 1-3 May 2024,

Vienna, Austria (2024).

[23] I. Stanković, O. Noel, and **M. Dašić**,
"Exploring influence of water on the friction on two dimensional surfaces",
MecaNano 2nd General Meeting, 1-3 May 2024,
Vienna, Austria (2024).

[24] **M. Dašić**, J. Fanfrlík, and J. Řezáč,
"Enhancing protein-ligand binding affinity via optimal selection of water molecules"
German Physical Society (DPG) Spring Meeting 2024, 17-22 March 2024,
Berlin, Germany (2024).

[25] **M. Dašić**, and I. Stanković,
"Molecular dynamics study on the impact of water distribution on nanoscopic friction in case of monolayer MoS2",German Physical Society (DPG) Spring Meeting 2024, 17-22 March 2024,
Berlin, Germany (2024).

[26] M. Jovanović, **M. Dašić**, and I. Stanković,
"The simulations of structural, thermodynamical, and mechanical characteristics of the mixture of ionic liquid and water using molecular dynamics: example of [bmim]+ [PF6]− ionic liquid",
German Physical Society (DPG) Spring Meeting 2024, 17-22 March 2024,
Berlin, Germany (2024).

[27] **M. Dašić**, and I. Stanković,
"Molecular Dynamics Investigation of the Nanoscopic Friction on Monolayer MoS2 in the Presence of Water",
STLE Annual Conference, Digital Proceedings, 21-25 May 2023,
Long Beach, California, United States of America (2023).

[28] **M. Dašić**, and I. Stanković,
"Influence of Water Quantity on the Nanoscopic Friction on Monolayer MoS2 Investigated with Molecular Dynamics",
The 8th European Nanomanipulation Workshop, 15-17 May 2023,
Krakow, Poland (2023).

[29] **M. Dašić**, and I. Stanković,
"Nanoscopic Friction on Monolayer MoS2 in Presence of Water Investigated with Molecular Dynamics",
German Physical Society (DPG) Spring Meeting 2023, 26-31 March 2023,
Dresden, Germany (2023).

[30] **M. Dašić**, I. Ponomarev, T. Polcar, and P. Nicolini,
"Tribological Properties of Selected Vanadium Oxides Investigated with ReaxFF molecular dynamics",
German Physical Society (DPG) Spring Meeting 2023, 26-31 March 2023,
Dresden, Germany (2023).

[31] **M. Dašić**, I. Ponomarev, T. Polcar, and P. Nicolini,
"Tribological Properties of Selected Vanadium Oxide Stoichiometries Studied with Reactive Molecular Dynamics",
11th International Conference of The Balkan Physical Union, 28 August - 1 September 2022,
Belgrade, Serbia (2022).

[32] **M. Dašić** and I. Stanković,
"Influence of the Size of Cation on the Structure and Tribological Properties of Ionic Liquids Studied with Molecular Dynamics",
11th International Conference of The Balkan Physical Union, 28 August - 1 September 2022, Belgrade, Serbia (2022).

[33] I. Stanković, **M. Dašić**, and C. García,
"Tubular structures of magnetic particles: platform for curvilinear nanomagnetism",
11th International Conference of The Balkan Physical Union, 28 August - 1 September 2022, Belgrade, Serbia (2022).

[34] I. Stanković, and **M. Dašić**,
"Non-equilibrium molecular dynamics investigation of a model ionic liquid lubricant for heavy-duty applications",
11th International Conference of The Balkan Physical Union, 28 August - 1 September 2022, Belgrade, Serbia (2022).

Радови у водећим међународним часописима (категорија М21а) - претходни период:

[35] I. Stanković, **M. Dašić**, J. A. Otálora, and C. García,
"A platform for nanomagnetism - assembled ferromagnetic and antiferromagnetic dipolar tubes",
Nanoscale 11, 2521 (2019).
doi: 10.1039/C8NR06936K

[36] K. Gkagkas, V. Ponnuchamy, **M. Dašić**, and I. Stanković
"Molecular Dynamics Investigation of a Model Ionic Liquid Lubricant for Automotive Applications",
Tribology International 113, 83-91 (2017)
doi: 10.1016/j.triboint.2016.12.017

[37] I. Stanković, **M. Dašić**, and R. Messina,
"Structure and Cohesive Energy of Dipolar Helices",
Soft Matter 12, 3056 (2016)
doi: 10.1039/C5SM02774H

Радови у водећим међународним часописима (категорија М21) - претходни период:

[38] **M. Dašić**, I. Stanković, and K. Gkagkas,
"Molecular Dynamics Investigation of the Influence of the Shape of Cation on the Structure and Lubrication Properties of Ionic Liquids",
Physical Chemistry Chemical Physics 21, 4375 (2019)
doi: 10.1039/C8CP07364C

Радови у међународним часописима (категорија М22) - претходни период:

[39] **M. Dašić**, K. Gkagkas, and I. Stanković,
"Influence of Confinement on Flow and Lubrication Properties of a Salt Model Ionic Liquid Investigated with Molecular Dynamics",
European Physical Journal E 41, 130 (2018)
doi: 10.1140/epje/i2018-11740-6

6. КВАНТИФИКАЦИЈА НАУЧНИХ РЕЗУЛТАТА КАНДИДАТА

Врста резултата	Вредност резултата (Прилог 2)	Укупан број резултата (укупан број резултата који подлежу нормирању)	Укупан број бодова (укупан број бодова након нормирања)
M21a+	20	1 (0)	20 (20)
M21a	12	2 (1)	24 (20.6)
M21	8	1 (0)	8 (8)
M22	5	1 (0)	5 (5)
M32	1.5	2 (0)	3 (3)
M34	0.5	27 (0)	13.5 (13.5)
УКУПНО			**73.5 (70.1)**

Поређење са минималним квантитативним условима за избор у тражено научно звање

Диференцијални услов за оцењивани период за избор у научно звање: виши научни сарадник	Неопходно	**Остварени нормирани број бодова**
Укупно	50	**70.1**
Обавезни: M11+M12+M21+M22+M23+M91+M92+M93	35	**53.6**

ПРИЛОГ 1

Претходни избори у звање

Република Србија
МИНИСТАРСТВО ПРОСВЕТЕ, НАУКЕ И ТЕХНОЛОШКОГ РАЗВОЈА
Матични научни одбор за физику

Број: 660-01-4/2020-14/8
27.03.2020. године
Б е о г р а д

На основу члана 27. став 1 тачка 1) и члана 76. став 5. Закона о науци и истраживањима („Службени гласник Републике Србије”, бр. 49/2019) и Правилника о поступку, начину вредновања и квантитативном исказивању научноистраживачких резултата истраживача („Службени гласник Републике Србије”, број 24/16, 21/17 и 38/17) и захтева који је поднео

Институт за физику у Београду

Матични научни одбор за физику на седници одржаној 27.03.2020. године, донео је

ОДЛУКУ
О СТИЦАЊУ НАУЧНОГ ЗВАЊА

Др Миљан Дашић
стиче научно звање
Научни сарадник

у области природно-математичких наука - физика

О Б Р А З Л О Ж Е Њ Е

Институт за физику у Београду

утврдио је предлог број 209/1 од 11.02.2020. године на седници Научног већа Института за физику у Београду и поднео захтев Матичном научном одбору за физику број 233/1 од 13.02.2020. године за доношење одлуке о испуњености услова за стицање научног звања **Научни сарадник.**

Матични научни одбор за физику на седници одржаној 27.03.2020. године разматрао је захтев и утврдио да именовани испуњава услове из члана 76. став 5. Закона о науци и истраживањима („Службени гласник Републике Србије”, бр. 49/2019) и Правилника о поступку, начину вредновања и квантитативном исказивању научноистраживачких резултата истраживача („Службени гласник Републике Србије”, број 24/16, 21/17 и 38/17) за стицање научног звања **Научни сарадник** па је одлучио као у изреци ове одлуке.

Доношењем ове одлуке именовани стиче сва права која му на основу ње по закону припадају.

Одлуку доставити подносиоцу захтева, именованом и архиви Министарства просвете, науке и технолошког развоја у Београду.

МИНИСТАР

Младен Шарчевић

МАТИЧНИ НАУЧНИ ОДБОР ЗА ФИЗИКУ
ПРЕДСЕДНИК

проф. др Милан Дамњановић

МИНИСТАРСТВО
НАУКЕ, ТЕХНОЛОШКОГ
РАЗВОЈА И ИНОВАЦИЈА
Матични научни одбор за физику
Број: 119-01-4/2024-03/33
22.11.2024.
Београд

На основу члана 27. став 1. тачка 1) и члана 76. став 5. Закона о науци и истраживањима („Службени гласник Републике Србије", бр. 49/2019) и Правилника о стицању истраживачких и научних звања („Службени гласник Републике Србије", број 159/2020 и 14/23) и захтева који је поднео Институт за физику у Београду, Институт од националног значаја за Републику Србију, Матични научни одбор за физику на седници одржаној 22.11.2024. године, донео је

ОДЛУКУ
О СТИЦАЊУ НАУЧНОГ ЗВАЊА

др Миљан Дашић
стиче научно звање
Научни сарадник
Реизбор
област Природно-математичке науке – Физика

О Б Р А З Л О Ж Е Њ Е

Институт за физику у Београду, Институт од националног значаја за Републику Србију

утврдио је предлог број 0801-2039/1 од 07.11.2024. године на седници Научног већа Института и поднео захтев Матичном научном одбору за физику број 0801-2039/2 од 07.11.2024. године за доношење одлуке о испуњености услова за реизбор у научно звање **Научни сарадник.**

Матични научни одбор за физику на седници одржаној 22.11.2024. године разматрао је захтев и утврдио да именовано лице испуњава услове из члана 76. став 5. Закона о науци и истраживањима („Службени гласник Републике Србије", бр. 49/2019) и Правилника стицању истраживачких и научних звања („Службени гласник Републике Србије", број 159/2020 и 14/23) за реизбор у научно звање **Научни сарадник** на основу чега је одлучио као у изреци ове одлуке.

Доношењем ове одлуке именовано лице стиче сва права која му на основу ње по закону припадају.

Одлуку доставити подносиоцу захтева, именованом лицу и архиви Министарства науке, технолошког развоја и иновација у Београду.

ПРЕДСЕДНИК МАТИЧНОГ НАУЧНОГ ОДБОРА

др Антун Балаж

МИНИСТАР

др Јелена Беговић

ПРИЛОГ 2

Руковођење пројектима

ÚOCHB AV ČR
IOCB PRAGUE
Ústav organické chemie a biochemie
Akademie věd České republiky, v. v. i.
Institute of Organic Chemistry and Biochemistry
of the Czech Academy of Sciences

Doc. RNDr. Jan Řezáč, Ph.D.
Senior scientist, team leader
e-mail: rezac@uochb.cas.cz

Prague, Dec 11 2024

Employment certificate – Dr. Miljan Dašić

To whom it may concern:

We certify that Dr. Miljan Dašić has worked at the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences (IOCB Prague) as a Postdoctoral Researcher in the period 1.3.2023 – 31. 10. 2024 and as an Associate Scientist in the period 1. 11. 2024 – 31. 12. 2024.

During his employment at IOCB Prague, Dr. Dašić participated in my team's project on the application of efficient quantum-mechanical calculations in computer-aided drug design. This project, running in the years 2021 – 2024, was internally funded by IOCB Prague. Dr. Dašić was leading the work in two work packages within the project:

1) Development and applications of software for automatic preparation of protein structures for quantum-mechanical scoring, and,

2) Development and applications of software for selecting structural water molecules which enhance protein-ligand binding affinity predictions.

The work on both topics included both scientific tasks in the field of computational chemistry of biomolecules and software development in Python.

In case of any further information needed, feel free to contact us.

Doc. RNDr. Jan Řezáč, Ph.D.

Flemingovo nám. 2
166 10 Praha 6
Czech Republic

+420 220 183 333
uochb@uochb.cas.cz
www.uochb.cz

IČ: 61388963
DIČ: CZ61388963

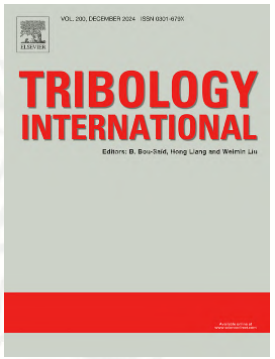
ПРИЛОГ 3

Рецензије радова

Miljan Dašić
https://orcid.org/0000-0002-1739-0784

Peer review (45 reviews for 17 publications/grants) Sort

- Review activity for **Algorithms.** (1)
- Review activity for **Applied sciences.** (9)
- Review activity for **Coatings.** (2)
- Review activity for **Energies.** (1)
- Review activity for **Fluids.** (1)
- Review activity for **Journal of sensor and actuator networks.** (1)
- Review activity for **Lubricants.** (7)
- Review activity for **Machines.** (5)
- Review activity for **Materials.** (6)
- Review activity for **Metals.** (1)
- Review activity for **Molecules.** (1)
- Review activity for **Optical and quantum electronics.** (1)
- Review activity for **Polymers.** (1)
- Review activity for **Sensors.** (1)
- Review activity for **Sustainability.** (2)
- Review activity for **Symmetry.** (1)
- Review activity for **Tribology international.** (4)



Tribology International

Certificate of Reviewing

Awarded for 5 reviews between August 2017 and March 2024
presented to

MILJAN DAŠIĆ

in recognition of the review contributed to the journal

The Editors of Tribology International

REVIEW CONFIRMATION CERTIFICATE

We are pleased to confirm that

Miljan Dašić

has reviewed 40 papers for the following MDPI journals in the period 2022–2026:

Algorithms, Lubricants, Applied Sciences, Machines, Molecules, Sensors, Energies, Coatings, Materials, Journal of Sensor and Actuator Networks, Sustainability, Fluids, Symmetry, Polymers, Metals

S. Tochev

Stefan Tochev, Chief Executive Officer
18 March 2026

MDPI

MDPI is a publisher of open access, international, academic journals. We rely on active researchers, highly qualified in their field to provide review reports and support the editorial process. The criteria for selection of reviewers include: holding a doctoral degree or having an equivalent amount of research experience; a national or international reputation in the relevant field; and having made a significant contribution to the field, evidenced by peer-reviewed publications.

Subject	**Thank you for submitting your Independent Review Report! - 1634637**
From	Frontiers in Chemistry Editorial Office
To	mdasic@ipb.ac.rs
Date	Fri 16:19

Dear Dr Dasic,

Thank you for submitting your independent review report for the manuscript "Water-Enhanced CO2 Capture in Metal-Organic Frameworks". The handling editor has been notified, and you can find a copy of your report below.

You will be informed once the interactive review process is activated, to allow direct discussion with the authors. Until this next stage, you can still modify your report if you have any outstanding comments.
You can access your report and the manuscript online using the following link:
https://review.frontiersin.org/review/bootstrap/d45d340f-cd59-4e9b-9a1a-d75b1ae85942

To familiarize yourself further with the Frontiers review guidelines:
https://www.frontiersin.org/Journal/ReviewGuidelines.aspx?s=3587&name=porous_crystalline_networks

Best regards,
Your Frontiers in Chemistry Team,

Frontiers | Editorial Office - Collaborative Peer Review Team
www.frontiersin.org
Avenue du Tribunal Fédéral 34
1005 Lausanne Switzerland

Subject **Congratulations on the article you reviewed - 1634637**

From Chemistry Production Office

To mdasic@ipb.ac.rs

Date Today 07:26

Hello, Dr. Dasic ,

Congratulations – the article that you recently reviewed: Water-Enhanced CO2 Capture in Metal-Organic Frameworks, by Jian Liu, Joseph Hupp, Randall Snurr, T Glover, Jaeden Cortés, Celine Cammarere, has now been published in Frontiers in Chemistry.

This article is an open-access publication, which means that it is accessible to any reader anywhere in the world. You can see it for yourself (and share it with your network) using this link: https://www.frontiersin.org/articles/10.3389/fchem.2025.1634637.

The article is also being disseminated onto the Frontiers research network (Loop).
Please ensure that your Frontiers profile on the Loop network is up-to-date by editing it here: http://loop.frontiersin.org/people/me

We want to hear about your experience with Frontiers. We are constantly striving to improve our peer review process, please complete our short 3-minute survey to tell us about your experience, your opinion is important and will guide future development
https://frontiersin.qualtrics.com/jfe/form/SV_9sfHMjCrBqCCUYe?survey=reviewerpub&Decision=Published&ArticleId=1634637&UserId=599033

Once again, congratulations. Your contribution really opens up your field for the entire world.

We look forward to your future submissions.

Thank you,
Frontiers in Chemistry Production Office
Chemistry.production.office@frontiersin.org
https://www.frontiersin.org/

SPRINGER NATURE

REVIEWER CERTIFICATE

This certificate is awarded to

Miljan Dašić

in recognition of their contribution to

1 manuscript in 2026 for

Tribology Letters

24 March 2026

Springer nature portfolio BMC Discover palgrave macmillan Birkhäuser Adis

ПРИЛОГ 4

Предавања по позиву

UNIVERSITY OF BELGRADE
Institute of Chemistry, Technology and Metallurgy
Institute of national importance for the Republic of Serbia
Njegoševa 12, 11001 Belgrade, P.O.B. 473, Serbia
Telephone: Exchange +381113640 230; Director +381113640 227; Fax: +381113640 234,
E-mail:ihtm@ihtm.bg.ac.rs; http://www.ihtm.bg.ac.rs

Belgrade, 03 June 2023

Invitation letter

COST CA21101 COSY Training School "Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications", **19 – 22 September 2023, Belgrade, Serbia**

To:
Dr Miljan Dašić
Institute of Organic Chemistry and Biochemistry
Czech Academy of Sciences

Dear Dr Dašić,

On behalf of the organizing committees, I am pleased to invite you to deliver an invited lecture at the **COST COSY Training School, "*Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications".*** This event is organized under the COSY COST Action (CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS, CA21101, https://cost-cosy.eu) for the first grant period and will take place in Belgrade, Serbia, from 19th to 22nd of September, 2023 (*https://www.trainingschool-cost-cosy.com*).

Please, let me know at your earliest convenience if you are willing to accept this invitation.

Looking forward to seeing you in Belgrade

Sincerely,

Sonja Grubisic

dr Sonja Grubišić
Research Professor,
IHTM-Center for Chemistry
University of Belgrade, Serbia
Email:sonja.grubisic@ihtm.bg.ac.rs

Scientific Organizing Committee:

María Pilar de Lara-Castells	Consejo Superior de Investigaciones Científicas - CSIC, Spain
Cristina Puzzarini	University of Bologna, Italy
Sonja Grubišić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy - ICTM, Serbia
Jiří Vaníček	Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland
Majdi Hochlaf	Université Gustave Eiffel, COSYS/IMSE, France
Francesca Mocci	University of Cagliari, Italy
Juan Carlos Hernández Garrido	Universidad de Cádiz, Spain

Local Organizing Committee:

Sonja Grubišić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Ivana Đorđević	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Dragan Popović	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Anita Lazić	University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy

Supported by:

Funded by the European Union

cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

COSY COST ACTION

Training School COST-COSY 2023, Belgrade

- CONFIRMED TRAINERS -

To achieve aims of the Training School we have a great team of eminent teachers from Spain, Switzerland, France, Italy, Romania, Sweden and Serbia.

READ MORE ABOUT COSY

MARÍA PILAR DE LARA-CASTELLS

Institute of Fundamental Physics of the Spanish National Research Council (IFF-CSIC), Madrid, Spain
(Intermolecular interactions and Clusters)

JIRI VANICEK

Ecole polytechnique fédérale de Lausanne, Lausanne, Switzerland
(Semiclassical Dynamics and Electronic Spectroscopy)

CRISTINA PUZZARINI

University of Bologna, Department of Chemistry "Giacomo Ciamician", Bologna, Italy
(Gas-phase Spectroscopy and Astrochemistry)

MAJDI HOCHLAF

Université Gustave Eiffel, COSYS/IMSE, Paris, France
(Intermolecular interactions, Clusters and Surfaces and Astrochemistry)

SONJA GRUBIŠIĆ

University of Belgrade, Institute of Chemistry, Technology and Metallurgy (ICTM), Belgrade, Serbia
(Grand Canonical Monte Carlo, Force Field development and MOFs)

MARTIN QUACK

Physical Chemistry, ETH Zurich, Zurich, Switzerland
(Quantum Dynamics, Symmetry, and Tunneling)

AATTO LAAKSONEN

Stockholm University, Division of Physical Chemistry, Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm, Sweden
(Modern Molecular Modelling and Simulations)

FRANCESCA MOCCI

University of Cagliari, UNICA, Department of Chemical and Geological Science, Cagliari, Italy
(Classical Dynamics and Coarse-grained models, Nucleic acids)

ANDREI NEAMTU

TRANSCEND Research Center Romania, Iasi, Romania
(Classical Dynamics, Biomolecules)

MILJAN DAŠIĆ

Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic;
Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia
(Classical and Reactive Molecular Dynamics)

VLADIMIR SREĆKOVIĆ

Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia
(Astrophysics and Physics of Ionosphere)

COST COSY

COST COSY Training School 2023
19-22 September 2023, Belgrade, Serbia

Teachers

María Pilar de Lara-Castells	Institute of Fundamental Physics of the Spanish National Research Council (IFF-CSIC), Madrid, Spain email: Pilar.deLara.castells@csic.es
Jiří Vaníček	Ecole polytechnique fédérale de Lausanne, Lausanne, Switzerland email: jiri.vanicek@epfl.ch
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Aatto Laaksonen	Stockholm University, Division of Physical Chemistry, Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm, Sweden email: aatto@mmk.su.se
Francesca Mocci	University of Cagliari, UNICA, Department of Chemical and Geological Science, Cagliari, Italy email: fmocci@unica.it
Andrei Neamțu	TRANSCEND Research Center Romania, Iasi, Romania email: andrei.neamtu@umfiasi.ro
Miljan Dašić	Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic; Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia email: mdasic@ipb.ac.rs
Vladimir Srećković	Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia email: vlada@ipb.ac.rs

THU, Sep 21	
9:30-11:00	**Martin Quack (Switzerland)** *"Molecules in motion: symmetries and primary processes between less than yoctoseconds and more than days"*
11:00-11:30	Coffee break
11:30-13:00	**Andrei Neamtu (Romania)** *"Sampling strategies for complex systems: enhanced-sampling simulations for the study of biomolecules"*
13:30-15:00	Lunch
15:00-16:30	Practice (Andrei Neamtu)
16:30-17:00	Coffee break
17:00-18:30	**Miljan Dašić (Czech Republic)** *"Computer-aided drug design"*

FRI, Sep 22	
9:30-11:00	**Jiří Vaníček (Switzerland)** *"Semiclassical dynamics and electronic spectroscopy"*
11:00-11:30	Coffee break
11:30-13:00	Practice (Miljan Dašić)
13:30-15:00	Lunch
15:00-17:00	*Poster session and coctail
17:00	**Closing addresses**
17:00-20:00	Free afternoon
20:00-	Social dinner

All lectures will take place in the Lecture Hall "Belgrade panorama" of Palace Hotel (6th floor).

*Poster session will be held in the Banquet Hall, 1st floor (Hotel Palace)

Computer-Aided Drug Design

Miljan Dašić [1,2]

[1]*Institute of Organic Chemistry and Biochemistry (IOCB), Czech Academy of Sciences (Prague, Czech Republic)*
[2]*Institute of Physics Belgrade (IPB), University of Belgrade (Belgrade, Serbia)*
mdasic@ipb.ac.rs

Advances in computational methods, in both hardware and software aspects, have revolutionized the field of drug discovery, making it possible to predict and optimize the interactions between small molecules (order of size: 10 - 100 atoms) and their target proteins (order of size: 1000 - 10000 atoms). This lecture aims to provide a comprehensive introduction into the multidisciplinary scientific discipline named **Computer Aided-Drug Design** (**CADD**) for an audience with diverse scientific backgrounds. In the ever-evolving efforts of pharmaceutical research, *CADD* has emerged as a fundamental discipline which combines the knowledge and insights of physics, chemistry, biology, and computer science. The key impact of *CADD* comes from speeding-up the drug discovery processes and reducing their experimental costs. Utilization of *CADD* belongs to the so called *in situ drug design*, which represents the first step of a long process - from designing potential drugs on a computer, over their clinical testing, and finally their approval and arrival to pharmacies, where patients can obtain them.

This lecture will consider the essential concepts, without overwhelming the audience with peculiar details. Throughout the 1.5 hour presentation, we will explain the key stages of the drug discovery process, from both experimental and computational point of view, emphasizing the *CADD*. Starting from an overview of molecular interactions and the role of proteins in disease pathways, we will explore the challenges of identifying suitable drug targets. The lecture starts by unraveling the foundational principles of molecular interactions, shedding light on the key role of proteins in diseases. Considering the target identification, students will gain insights into the crucial task of pin-pointing proteins that serve as potential drug targets. As the lecture unfolds, the focus moves toward molecular docking, which is a cornerstone of *CADD*. We will highlight the significance of molecular docking, in which computer simulations predict how do potential drugs interact with their target proteins. After providing a general theoretical background, we will move forward by presenting selected research studies done in the Department of Noncovalent Interactions of the *IOCB* in *Prague*, *Czech Republic*. Through different illustrative examples, students will get to know how computer simulations predict the binding affinities between drug candidates and target proteins. The procedure called *scoring* is essential for ranking the studied drug candidates, and hence selecting the most promising ones. We will provide a brief introduction into the physics-informed scoring methods developed and employed in the research studies done at the *IOCB* in *Prague*. Within the field of *CADD*, there are two principally different approaches: *Ligand-Based Drug Design* (*LBDD*) and *Structure-Based Drug Design* (*SBDD*). Since the lecturer's research group at the *IOCB* in Prague works mainly within the framework of *SBDD*, the key processes of *SBDD* will be presented, including:

1. *Protein Structure Determination* - The process starts by determining the 3D structure of the target protein using experimental techniques like X-ray Crystallography or Nuclear Magnetic Resonance (*NMR*). By using those experimental techniques, it is possible to

obtain a detailed information about the protein's active site, where drug binding occurs. Visualization on a computer (e.g., using the software named PyMOL) can help in designing the drug candidates.

2. *Ligand Screening* - Potential drug molecules, usually referred to as ligands, are virtually screened or experimentally tested to identify those that could potentially interact with the target protein's active site.
3. *Molecular Docking and Scoring* - Computational tools simulate how do ligands bind to protein's active site, predicting their binding orientations, non-covalent interactions and affinities. This helps in selecting the most promising drug candidates.
4. *Lead Optimization* - Based on the docking results, chemists modify the structure of selected ligands in order to enhance their binding affinities with the target protein. Furthermore, iterative cycles of design, synthesis, and testing, refine the compounds' physico-chemical properties (e.g., solubility).
5. *Validation* - Promising compounds are synthesized and experimentally tested to confirm their predicted target binding and biological activity. This process helps in bridging the gap between the computational predictions and the real-world biochemical behavior of the drug candidates.
6. *Clinical Development* - Compounds that demonstrate strong binding affinity, desirable pharmacological properties, as well as safety characteristics, move into the clinical trials, which represent a critical step in bringing potential drugs to the pharmacies.

The power of *SBDD* lies in its ability to rationally design drug candidates that align with the complex molecular landscape of diseases. By visualizing and understanding their physico-chemical interactions, researchers can develop molecules that selectively modulate target proteins, at the same time reducing unwanted side effects and increasing the therapeutic efficiency. Structure-Based Drug Design relies on the synergy of physics, chemistry, biology, and computer science. In a nutshell, *SBDD* is an approach that transforms static protein structures into dynamic tools for guiding the discovery of next-generation medicines. Through a symbiosis of cutting-edge technology and scientific insights, *SBDD* accelerates the drug discovery process, directing us closer to the realization of precision therapies for a range of medical challenges. Speaking about the cutting-edge technology, we refer to the advanced hardware (i.e., High Performance Computing (*HPC*) resources) and to the advanced software (development of *CADD* software in high-level object oriented programming languages, mainly in Python).

In conclusion, this introductory lecture on *Computer Aided-Drug Design* aims to explain the complexities of the field, thus offering a good starting point for master and doctoral students coming from diverse scientific backgrounds. As we point out the strong synergy between physics, chemistry, biology, and computer science, participants coming from any of those scientific disciplines will understand what could be their role, in case they choose to orient their scientific path in the direction of *CADD*. Expectedly, the field of *CADD* incorporates a strong interplay between academic research and industrial research and development (*R&D*) sector, mainly of the pharmaceutical and medical industries.

Subject	**Poziv za gostovanje na dogadjaju “Dani fotonike”**
From	Николина Братић
To	mdasic@ipb.ac.rs
Cc	uofbelgradeosastudentchapter@gmail.com
Date	2023-12-06 13:49

Poštovani Miljane Dašiću,

Moje ime je Bratić Nikolina i pišem Vam ispred organizacionog tima događaja "Dani Fotonike" koji će se održati 26. i 27. decembra na Elektrotehničkom fakultetu Univerziteta u Beogradu, u organizaciji Optica student chapter Univerziteta u Beogradu.

Zadovoljstvo mi je da Vas ispred organizacije pozovem da budete jedan od govornika na našem događaju. Prepoznali smo Vaš izuzetan doprinos u oblasti fotonike i smatramo da biste bili inspirativan govornik za sve zainteresovane studente našeg Univerziteta. Ukoliko ne budete u mogućnosti da fizički prisustvujete događaju, rado bismo Vam omogućili da se predstavite putem MS Timsa.

Tema Vašeg govora može obuhvatiti Vaše istraživačko iskustvo u oblasti fotonike i put koji ste prešli do svoje trenutne pozicije. Smatramo da Vaša priča može biti izuzetno inspirativna za studente i ostale učesnike događaja. Cilj ovog skupa je popularizacija fotonike u Srbiji, a Vaše iskustvo i znanje bi sigurno doprineli ostvarenju tog cilja.

Molimo Vas da nam potvrdite svoju dostupnost i interesovanje za učešće u najkraćem mogućem roku, kako bismo pravilno isplanirali raspored govornika i logistiku događaja.

Ukoliko imate dodatna pitanja ili Vam je potrebno više informacija, slobodno me kontaktirajte.

Radujemo se Vašem učešću na "Danima Fotonike" i deljenju Vašeg znanja sa našom zajednicom!

S poštovanjem,

Bratić Nikolina
Oraginizacioni tim "Dani fotonike"
Optica Student Chepter Univerziteta u Beogradu
0654674656
bn210130d@student.etf.bg.ac.rs

DANI FOTONIKE
26–27.12.2023.

UPOZNAJ SE SA CELIM SPEKTROM MOGUĆNOSTI!

- Kvantni Računari
- Biosenzori
- Bioreaktori
- Integrisana Fotonika
- Spektroskopija
- Karijerni put u fotonici

Registruj se kako bi prisustvovao događaju!

OPTICA
Formerly OSA

26.12. u 18-20h

Sala 55

Milan Mašanović
Freedom Photonics

Ozren Petrović
LIGENTEC

Milan Sinobad
DESY

Marija Trajković
Eindhoven Hendrik Casimir Institute

Biljana Stankov
IPB

27.12. u 18-20:30h

Sala 59

Miljan Dašić
IOCB Prague

Željko Janićijević
Helmholtz-Zentrum Dresden-Rossendorf

Milana Lalović
CERN

Radoica Draškić
Tenderly

Isidora Teofilović
DTU Photonics

Marina Radulaški
UC Davis

26.12. u 17h sala 65

PANEL SESIJA

Izazovi u fotonici: Akademija VS Industrija

Učesnici:

Specijalni gosti iz naše i strane industrije i akademije!

UNIVERSITY OF BELGRADE
Institute of Chemistry, Technology and Metallurgy
Institute of national importance for the Republic of Serbia
Njegoševa 12, 11001 Belgrade, P.O.B. 473, Serbia
Telephone: Exchange +381113640 230; Director +381113640 227; Fax: +381113640 234,
E-mail:ihtm@ihtm.bg.ac.rs; http://www.ihtm.bg.ac.rs

Belgrade, 08 January 2024

Invitation letter

COST CA21101 COSY 1st WG2 Virtual Meeting
***"From quantum to classical dynamics of isolated molecules and 3D materials", February 6 2024,* Belgrade, Serbia**

To:
Dr Miljan Dašić
Institute of Organic Chemistry and Biochemistry
Czech Academy of Sciences

Dear Dr Dašić,

On behalf of the organizing committees, I am delighted to invite you to deliver an invited talk at the **COST COSY WG2 Virtual Meeting *"From quantum to classical dynamics of isolated molecules and 3D materials".*** This event is organized within the framework of the COSY COST Action (CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS, CA21101, https://cost-cosy.eu) for the second grant period and will take place on February 6, 2024.

We would greatly appreciate your contribution and kindly ask to confirm at your earliest convenience, if you are willing to accept this invitation.

Looking forward to your participation.

Sincerely,

Sonja Grubišić

dr Sonja Grubišić
Research Professor,
IHTM-Center for Chemistry
University of Belgrade, Serbia
Email:sonja.grubisic@ihtm.bg.ac.rs

Scientific Organizing Committee:

María Pilar de Lara-Castells	Consejo Superior de Investigaciones Científicas - CSIC, Spain
Cristina Puzzarini	University of Bologna, Italy
Sonja Grubišić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy - ICTM, Serbia
Jiří Vaníček	Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland
Majdi Hochlaf	Université Gustave Eiffel, COSYS/IMSE, France
Francesca Mocci	University of Cagliari, Italy
Juan Carlos Hernández Garrido	Universidad de Cádiz, Spain
Vladimir Srećković	Institute of Physics Belgrade, University of Belgrade, Serbia

Local Organizing Committee:

Sonja Grubišić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Ivana Đorđević	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Dragan Popović	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Snežana Spasić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy

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COSY COST ACTION

CONTENT

Phonon-Inspired Normal Dynamics of Lattices

Miljan Dašić[1,2], Antonio Cammarata[1], Paolo Nicolini[1,3]

[1]*Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, 16627 Prague, Czech Republic,*
[2]*Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia,*
[3]*Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 18200 Prague, Czech Republic*

Normal Dynamics (*ND*) is a simulation technique providing a way to integrate the Newton's classical mechanics equations of motion, by adequately sampling the reciprocal space. Appropriate sampling strategies and their capability of producing dynamical trajectories at the *ab initio* level on an ordinary desktop computer will be discussed. *ND* enables to: (1) obtain a systematic improvement of the accuracy, and fine tune the computational load, and (2) take into account the atomic distortions happening across large distances, without the need of using large unit cells. Theoretical background of the *ND* method (which is based on phonons [1]) will be presented, together with several case studies which illustrate the method's applicability. Also, it will be explained that this simulation technique is general and it can be used for simulating periodic, semiperiodic and finite systems, such as crystals, slabs, or molecules. Authors have implemented the *ND* method in the *Fortran* programming language, and named the developed software - *PINDOL* (Phonon-Inspired Normal Dynamics of Lattices). *PINDOL* is an open-source software package for performing atom dynamics in the NVE and NVT ensembles [2].

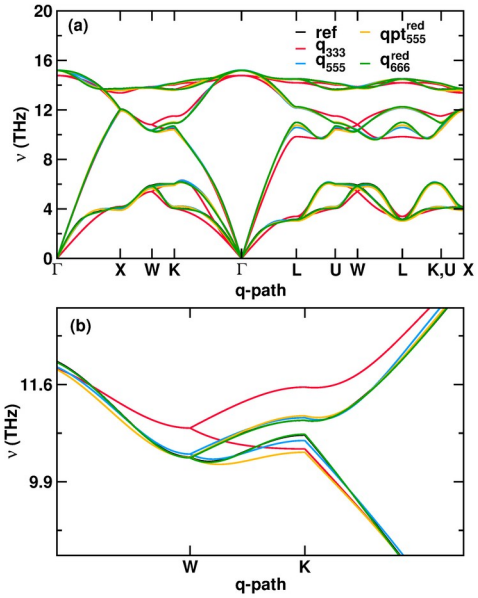

Fig 1. (a) Phonon band structure of crystalline silicon obtained with the frozen phonon approach (ref) and extracted from the effective force constants at 10 K in different sampling sets. (b) Detail of the band structures in (a).

References:

1. D. M. Wallace, Thermodynamics of Crystals, John Wiley & Sons Inc (1972), USA [book].
2. Link to the *PINDOL* project: https://github.com/acammarat/pindol.

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Dr Miljan Dašić
Institute of Organic Chemistry and Biochemistry

Czech Academy of Sciences

in Zemun, November 13th, 2024

Dear Dr Dašić,

It is my great pleasure to invite you, as a represent of your academic institution (Institute of Organic Chemistry and Biochemistry (IOCB Prague) of the Czech Academy of Sciences, Prague, Czech Republic), to present your work and accomplished results regarding the applications of Semi-empirical Quantum Mechanical (SQM) methods in modeling protein-ligand interactions at Training Events No. 6, No. 7, and No. 8 in the framework of our EU-funded project.

Your expertise from IOCB Prague highly resonates with the EU Horizon Doctoral Network - BLESSED: Bridging Models at Different Scales to Design New Generation Fuel Cells, which will be held at Université de Picardie Jules Verne, Amiens, France in the period 25th-27th November 2024.

I hope that you can accept this invitation, and I am looking forward to welcoming you in Amiens, France, where you will share your expertise gained at IOCB Prague with other colleagues in our Network.

Yours sincerely,

Dr Igor Stankovic

Principal Research Fellow
Institute of Physics Belgrade
tel. +381 65 601 9974
http://www.ipb.ac.rs/

BLESSED
Electrified mobility

BLESSED: Bridging Models at Different Scales To Design New Generation Fuel Cells for Electrified Mobility

Training Events No. 6, No. 7 and No. 8

25-27 November 2024, UPJV, Amiens, France

First Day (25/11)

Time	Content	Who
13:00 – 13.30	Welcome	ALL
13.30 – 15.00	How do we realize molecular dynamics models in LAMMPS? Design of simulation.	Igor Stanković
15.00 – 15.30	Coffee break	
15.30 – 17.00	How to include quantum effects into molecular dynamics simulations.	Jens Poulsen

Second Day (26/11)

Time	Content	Who
09.00 – 10.30	Introduction to phase-field models	Jens Poulsen
10.30 - 11.00	Coffee break	
11.00 – 12.30	Semi-empirical quantum-mechanical (SQM) methods for modeling molecular interactions	Miljan Dašić
12.30 – 13.30	Lunch break	
13.30– 15.00	Modeling of manufacturing processes	Alejandro A. Franco
15.00 – 15.30	Coffee break	
15.30 – 17.00	Modeling approaches for electrochemical energy devices – Part I	Francisco Fernandez

19:00 or 19.30 - Dinner in the city center (google maps link)

Third Day (27/11)

Time	Content	Who
09.00 – 10.30	Modeling approaches for electrochemical energy devices – Part II	Diego Galvez Aranda
10.30 - 11.00	Coffee break	
11.00 – 12.30	Validated Examples for Modelling the Manufacturing of Electrochemical Energy Devices	Mohammed Alabdali
12.30 – 13.30	Lunch break	
13.30 – 15.00	Virtual Reality Practices	Soorya Saranavan and Utkarsh Vijay
15.00 – 15.30	Coffee break	
15.30 – 17.00	Virtual Reality Practices	Soorya Saranavan and Utkarsh Vijay

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Argentinian-Serbian Nanotechnology Workshop

Challenges in bridging theory and experiments

Institute of Physics Belgrade, the reading room of the library dr Dragan Popović

Friday, November 22nd, 2024, 10:00-12:30

time	topic/presenter
10:00	**Modeling interaction of small molecules with materials: friction forces, intercalation, and memory effects** *Dr Igor Stankovic* Senzor Infiz / Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
10:35	**Unveiling the Pathways: KPFM and Modeling Insights into MoS_2 Nanosheet Network Behavior in Transistor Devices** *Dr Jelena Pešić* Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben, Austria
11:10	**Low-Energy Ion-Surface Interactions: From Spectral Anomalies to Charge Transfer Mechanisms** *Dr Fernando J. Bonetto* Surface Physics Group, Institute of Physics of Littoral (CONICET-UNL), Güemes 3450, S3000GLN Santa Fe, Argentina.
11:45	**Semi-empirical quantum-mechanical (SQM) methods for modeling molecular interactions** *Dr Miljan Dašić* Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo náměstí 2, 166 10 Prague, Czech Republic Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

organized by: Dr Miljan Dašić, Dr Igor Stanković, Dr Jelena Pešić

Modeling interaction of small molecules with materials: friction forces, intercalation, and memory effects

Dr Igor Stanković

Senzor Infiz / Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Molecular dynamics (MD) simulations have become an invaluable tool for investigating and predicting the behavior of small molecules in complex environments, providing insights into their structural, thermodynamic, and transport properties. This talk will highlight recent advancements in using MD to understand molecular interactions in diverse systems, including phosphonium-based ionic liquids [1], aluminum fluoride intercalation in graphite for battery applications [2], and water clusters in nanoscale geometries [3]. First, we explore the impact of water content on the dynamic properties of phosphonium ionic liquids, revealing how water molecules modulate ion interactions and impact viscosity, diffusion, and thermal stability. Next, we examine the role of AlF3 in rechargeable aluminum batteries, using MD to uncover the mechanisms behind its intercalation in graphite and implications for energy storage optimization. Finally, we delve into the behavior of water clusters on graphene nanoribbons under varying electric fields, showcasing MD's capability to capture ferroelectric effects relevant to future nanotechnology applications. By illustrating these cases, this talk will emphasize MD's role in elucidating the fundamental mechanisms behind small molecule interactions in complex systems, guiding the design and optimization of materials across energy storage, nanotechnology, and beyond.

[1] I. Stanković, M. Dašić, M. Jovanović, A. Martini, Langmuir 2024, 40, 17, 9049–9058.

[2] S.J. Rodríguez, A.E. Candia, I. Stanković, M.C.G. Passeggi, G.D. Ruano, ACS Appl. Nano Mater. 2023, 6, 18, 16977–16985.

[3] arXiv:2304.09738

Unveiling the Pathways: KPFM and Modeling Insights into MoS_2 Nanosheet Network Behavior in Transistor Devices

Dr Jelena Pešić

Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade

Chair of Physics, Department Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben

In this talk, we will explore how Kelvin Probe Force Microscopy (KPFM) and a tailored network model reveal the complex behavior of MoS_2 nanosheet networks in transistor devices. Using in-operando KPFM, we image the potential distribution across MoS_2 networks, isolating potential drops at nanosheet junctions and mapping how these affect current paths. This imaging highlights distinct types of junctions within the network, emphasizing the impact of overlap and trapped impurities on resistance. We develop a model that simulates the formation of current pathways across these nanosheet networks, correlating conductive regions to the overall device morphology and conductivity.

Our findings suggest that current flow often follows the path of least resistance, confirming the “winner-takes-all” behavior documented in similar systems. The model further quantifies the likelihood of current pathway formation, supporting a more detailed understanding of connectivity within these networks. Ultimately, this study bridges microscopic KPFM observations with macroscopic device properties, helping build strategies for enhancing network connectivity and optimizing device performance in applications of solution-processed 2D materials. [1]

[1] **Imaging Junctions in Two-Dimensional Semiconductor Nanosheet Network Transistors**, Jelena Pešić, Simon Leitner, Joseph Neilson, Igor Stanković, Muhammad Zubair Khan, Dragana Tizić Matković, Adam G. Kelly, Tian Carey, Jonathan Coleman, Aleksandar Matković, *under review.*

Semi-empirical quantum-mechanical (SQM) methods for modeling molecular interactions

Dr Miljan Dašić

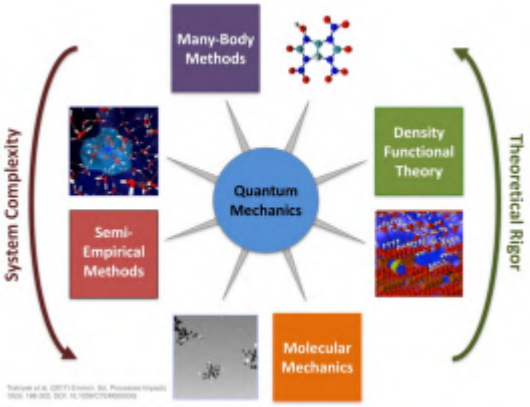
Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences,
Flemingovo náměstí 2, 166 10 Prague, Czech Republic

Scientific Computing Laboratory, Center for the Study of Complex Systems,
Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, Serbia

Semi-empirical quantum mechanical (SQM) methods represent computational techniques used to model molecular interactions implementing a balance of accuracy and computational efficiency [1]. Unlike fully ab-initio methods that exclusively rely on quantum mechanical calculations, SQM methods include empirical data [2], such as: ionization potentials, electron affinities, and orbital energies from experimental sources. These parameters simplify calculations by approximating certain electron interactions, thus providing insights into electronic structure, binding energies, and molecular geometries for larger systems, where purely quantum mechanical treatment would be computationally too expensive, or even prohibitive.

In case of research regarding hydrogen fuel cells, SQM methods provide complementary insights to primary methods, such as Density Functional Theory (DFT), which is often used for detailed studies, especially in catalysis. While DFT provides precise descriptions of chemical processes, SQM is a valuable tool for estimating binding energies in fuel cell catalysts, for studying interaction energies in polymer electrolyte membranes, and for analyzing adsorption on catalytic surfaces where computational speed is a priority. By applying SQM either as a preliminary tool or integrated within hybrid models, it is possible to explore broader molecular configurations and interactions of fuel cell components, hence coupling efficient initial studies with higher-accuracy studies. Such a flexibility makes SQM useful in preliminary screenings, where large datasets and complex systems need to be handled fastly.

As the lecturer Dr Dašić is actively conducting research based on a specific SQM approach, namely the SQM2.20 scoring function which is used in determining Protein-Ligand binding affinity predictions [3], one part of the lecture will cover that topic.



Rerefences

[1] Dral, Pavlo O., ed. Quantum Chemistry in the Age of Machine Learning. Elsevier, **2022**.
[2] Stewart, James JP., Journal of Molecular modeling **2007**, 13, 1173.
[3] Pecina, A.; Fanfrlík, J., Lepšík, M., Řezáč, J., Nature Communications **2024**, 15, 1127.

Low-Energy Ion-Surface Interactions: From Spectral Anomalies to Charge Transfer Mechanisms

Fernando J. Bonetto

Surface Physics Group, Institute of Physics of Littoral (CONICET-UNL), Güemes 3450, S3000GLN Santa Fe, Argentina.

The Surface Physics Group of Santa Fe (Argentina) specializes in characterizing surfaces and 2D materials through advanced techniques, including STM, AFM, AES, EELS, and LEIS, combined with theoretical models. This presentation will focus on three recent studies conducted in our group on low-energy ion interactions with surfaces.

The first study explores unexpected peaks in the LEIS spectra of Ar+ ions scattered from a Cu(111) surface, which cannot be explained by the standard binary collision model. Using molecular dynamics simulations, we show that these spectral features arise from surface defects such as islands or steps, demonstrating the impact of imperfections on LEIS spectra. Next, we investigate charge transfer in collisions between hydrogen ions and C60-based carbon films deposited on Cu(111). The study reveals how substrate atoms and electronic structure of the grown films influence the charge transfer process depending on film thickness.

Finally, we present novel measurements of neutral and ion fractions of Ne+ions backscattered by MoS_2 and metallic Mo surfaces. Despite the distinct electronic properties of the two targets, neutralization rates remain high across various energies and collision angles. Theoretical calculations indicate that resonant charge transfer is more prominent in MoS_2, while Auger neutralization dominates for metallic Mo. The discrepancy between experimental and calculated neutral fractions is attributed to excited states in Ne projectiles. These findings offer new insights into ion-surface interactions and enhance our understanding of charge transfer mechanisms in low-energy collisions.

Workshop on Integrating Simulations and Experiments for Advanced Applications

During the meeting, the latest results of research and industrial activities within the EU-funded projects **BLESSED**, **ULTIMATE-I**, and **HIP-2d-QM** will be presented, with a focus on:

- **fuel cells and functional materials**,
- **advanced simulation methods**,
- **textiles for optical and space applications**.

The working language of the meeting is **English**.

The meeting will take place
on **Tuesday, January 13, 2026**, from **9:30 a.m. to 12:30 p.m.**
in **Hall 3, 1st floor, SANU Palace**,
35 Knez Mihailova Street, Belgrade.

Organized by: Dr Miljan Dašić, Dr Igor Stanković, and Dr Jelena Pešić.

time	topic/presenter
9:30	**Registration**
10:00	**Welcome to the Institute of Technical Sciences SASA** *Lidija Mančić*
10:10	ULTIMATE-I project **ReaxFF for modeling the interaction of water with graphene edges** *Igor Stanković* Institute of Physics Belgrade and Senzor Infiz, Belgrade, Serbia
10:25	2D-HIP-QM project **Engineering Current Paths in MoS_2 Nanonetworks for Thin-Film Electronics** *Jelena Pešić* Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia, and Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben, Austria
10:40	ULTIMATE-I project **Textile mirrors for space applications** *Carlos Garcia* Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
10:55	**Coffee Break**

time	topic/presenter
11:00	BLESSED project **Multiscale Modeling of Enzyme-Substrate Interactions** *Dr Miljan Dašić* J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Dolejškova 2155/3, 182 00 Prague 8, Czech Republic Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
11:15	BLESSED project **Understanding Electrode Fabrication and Carbon Degradation in PEMFCs Studies using Density Functional Theory and Discrete Element Method Simulations** Matilde Russo[1,3], Sourab Barath Vijayaraghavan[1,2], Peter Lindstedt [3], Alejandro A. Franco[1,2], Matthias Baldofski[1] [1] Freudenberg Technology Innovation SE & Co. KG, 69469 Weinheim, Germany, [2] Université de Picardie Jules Verne, F - 80039, Amiens Cedex 1, France Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, Hub de l'Energie, 15 rue Baudelocque, 80039, Amiens Cedex, France, [3] Imperial College London, Exhibition Road, South Kensington, London SW72AZ, UK
11:45	BLESSED project **Hydration-Controlled Water Network Formation and Density in Crystalline and Amorphous Nafion Membranes** Mateja Jovanović[1,2,3], Nicolas Bernhard[1], Matthias Baldofski[1], Marcin Rybicki[1,4], Miljan Dašić[3], Igor Stanković[3,5] [1] Freudenberg Technology Innovation SE&Co., Weinheim, Germany, [2]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts(SASA), Belgrade, Serbia, [3] Institute of Physics, University of Belgrade, Zemun, Serbia, [4] Freudenberg e-Power Systems GmbH, München, Germany [5]Departamento de Ingenería Mecánica, Universidad Técnica Federico Santa María, Valparaíso, Chile
12:00	**Concluding remarks and discussion**

ПРИЛОГ 5

Публикације категорије М34

Dresden 2026 – scientific program

MM: German Association of Metal and Materials Physics

MM 32: Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I

MM 32.5: Lecture

Thursday, March 12, 2026, 12:15–12:30, SCH/A251

Selection status for this post: Title, author's block and summary

Mechanical Behaviour of Nafion Membranes — •Mateja Jovanovic[1,2,3], Matthias Baldofski[2], Nicolas Bernhard[2], Marcin Rybicki[2,4], Miljan Dasic[3], and Igor Stankovic[3,5] — [1]Institute of Technical Sciences of the SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — [2]Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [3]Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — [4]Freudenberg e-Power Systems GmbH, Bayerwaldstrasse 3, 81737 München, Germany — [5]Departamento de Ingeneria Mecanica, Universidad Tecnica Federico Santa Maria, Av. Espana 1680, Valparaiso, Chile

Proton Exchange Membrane Fuel Cells (PEMFCs) utilise polymer membranes like Nafion, valued for their proton conductivity and mechanical integrity. In this work, we examine the stress-strain response of Nafion membranes, focusing on how hydration, crystallinity, and temperature modulate mechanical behavior, using molecular dynamics simulations. Here, we demonstrate that membrane hydration level and structural ordering fundamentally influence mechanical properties under applied stress. Water distribution and polymer chain dynamics are closely connected to the stress-strain response, suggesting that structural organization at the nanoscale is crucial in governing overall mechanical performance across different conditions. By integrating clustering algorithms, structural descriptors, and stress-strain analyses, this study provides a comprehensive view of how membrane architecture and environmental factors govern mechanical performance.

Keywords: Nafion; Proton Exchange Membrane; Molecular Dynamics; Mechanical Properties; Stress-Strain Response

Dresden 2026 – scientific program

BP: Professional Association for Biological Physics

BP 2: Computational Biophysics I

BP 2.5: Presentation

Monday, March 9, 2026, 10:30–10:45, BAR/0106

Selection status for this post: Title, author's block and summary

Multi-Scale Computational Framework for Modeling Metabolic Pathways — • Milјan Dašić , Ashwathi Poolamanna , Mehrnoosh Khodam Hazrati , and Štěpán Timr — J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences, Dolejškova 2155/3, 182 00 Prague 8, Czech Republic

Spatial organization of enzymes (clustering, assemblies, and substrate channeling) has been increasingly recognized as a key determinant of metabolic efficiency. Recent studies suggest that non-specific enzyme-substrate interactions and molecular crowding can further impact the performance of metabolic pathways. However, the combined effect of these factors remains insufficiently quantified.

To address this gap, we developed a multi-scale computational framework connecting molecular-level enzyme-substrate interactions with emergent pathway-level kinetics. We first perform extensive coarse-grained Molecular Dynamics (MD) simulations with LAMMPS to quantify substrate transition kinetics at varying crowding levels. Resulting trajectories are analyzed using Markov State Models (MSMs) to extract the relevant states and transition rates. These kinetic parameters are then used to parameterize stochastic Reaction-Diffusion (RD) simulations in Smoldyn, enabling the study of large enzyme assemblies, different reaction orders, and multi-step metabolic pathways.

Our results reveal how molecular interaction strengths, crowding conditions as well as enzyme spatial organization impact pathway efficiency across scales: from nanometers and nanoseconds (MD) to micrometers and seconds (RD).

Keywords: coarse-grained molecular dynamics; stochastic reaction-diffusion simulations; enzymes; substrates; metabolic pathways

International Union of Pure and Applied Physics (IUPAP) Conference

XXXVI IUPAP Conference on Computational Physics (CCP2025)

November 03 – 07, 2025

Virtual only conference
Oak Ridge, Tennessee

The IUPAP Conference on Computational Physics is an annual international conference that covers all aspects of computational physics. The conference rotates on a triannual cycle between Europe/Africa, Asia and the Americas. In 2025 the conference is hosted by Oak Ridge National Laboratory in Oak Ridge, Tennessee as a virtual only event.

This conference will highlight advances in applications, algorithms and implementations of computational approaches in all areas of physics except quantum computing.

1. Condensed Matter Physics / Materials
2. Statistical Mechanics
3. Many Body Physics
4. Soft Matter and Polymers
5. Biophysics
6. Fluid Dynamics and Continuum Mechanics
7. Plasma Physics and Fusion
8. Nuclear and Particle Physics
9. Astrophysics, Cosmology and Gravitation
10. Algorithms and Novel Hardware Scientific Computing
11. Applications of Machine Learning and Artificial Intelligence

Book of Abstracts

26th IUPAP Conference of Computational Physics

Oak Ridge National Laboratory

2025

https://ccp2025.ornl.gov

1.7: Impact of Water Content on the Mechanical and Thermodynamic Properties of Phosphonium Ionic Liquids

Monday, 8:10am, Breakeout 2

Miljan Dašić, Igor Stanković, Mateja Jovanović, Ashlie Martini

Affiliation of Miljan Dašić, Igor Stanković, and Mateja Jovanović: Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Belgrade (Serbia)

Affiliation of Ashlie Martini: Department of Mechanical Engineering, University of California Merced, Merced, California (United States of America)

Submitted by:*Miljan Dašić; mdasic@ipb.ac.rs; Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Belgrade (Serbia)*

Phosphonium-based Room-Temperature Ionic Liquids (RTILs) have been gaining an increasing attention due to their unique physicochemical properties, which make them suitable for applications regarding lubrication, electrochemistry, and green chemistry. However, their behavior is significantly influenced by the water content, which alters their mechanical and thermodynamic properties. Taking this fact into account, we conducted extensive All-Atom Molecular Dynamics simulations, in order to investigate how varying water content affects the transport and thermodynamic properties of the three representative phosphonium-based RTILs. By analyzing the structural, transport, as well as energetic characteristics of these ionic liquids, we provide detailed insights into the fundamental mechanisms governing their dynamic behavior in the presence of water.

Our study focuses on the key transport properties, such as viscosity and self-diffusion coefficients, and their dependence on water concentration. We have observed that increase of water content significantly enhances ion mobility by disrupting ion-ion interactions. Water molecules preferentially interact with ionic species, hence effectively reducing Coulombic interactions and hydrogen bonding networks within the ionic liquid. This weakening of electrostatic forces leads to: a noticeable decrease in viscosity, and also to a noticeable increase in diffusion coefficients, thus highlighting the critical role of water content in these systems.

Additionally, we examined the thermodynamic stability of the studied ionic liquids mixed with water by analyzing interaction energies and phase behavior. Presence of water leads to a decrease

of cohesive energy density, hence resulting in a lower boiling point and increased volatility, compared to the boiling point and volatility of a pure ionic liquid. These findings suggest that phosphonium-based ionic liquids exhibit a water-dependent transition of their structure, which influences their macroscopic properties.

Results regarding phosphonium ionic liquids were compared with the well-studied 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim]+ [PF6]-) ionic liquid, which was used as a reference. Our comparative analysis revealed that phosphonium ionic liquids exhibit distinct water interaction patterns due to their larger, more hydrophobic cation structure. This distinction provides critical insights into their suitability for specific applications where water tolerance or exclusion is required.

Our study underscores the importance, and even necessity, of considering the water content when designing and selecting phosphonium ionic liquids for practical applications. Besides that, our findings significantly contribute to the broader understanding of how do molecular-scale interactions govern the macroscopic properties of ionic liquids, tracing the way for improved formulations tailored for industrial applications of ionic liquids in the fields like: tribology, solvent design, electrochemistry, etc. By elucidating the intricate role which water plays in mixtures with phosphonium ionic liquids, our work provides a foundation for optimizing the performance of such RTILs in various scientific and engineering/technological fields.

1.30: Correlation Between Nanoscale Crystallinity, Density, and Hydration in Nafion Membranes: Experimental and Molecular Dynamics Insights

Monday, 11:20am, Breakeout 2

Mateja Jovanović Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany Institute of Technical Sciences of the Serbian Academy of Sciences and Arts (SASA), K. Mihailova 35/IV, 11000 Belgrade, Serbia Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Dr. Nicolas Bernhard, Matthias Baldofski, Dr. Marcin Rybicki Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany

Dr. Miljan Dašić, Dr. Igor Stanković Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Submitted by:*Mateja Jovanović; mateja@ipb.ac.rs; Junior Research Assistant*

Proton Exchange Membrane Fuel Cells (PEMFCs) represent one of the candidate technologies for sustainable energy conversion. Nafion is considered a benchmark polymer membrane material due to its high proton conductivity and mechanical stability. However, its performance is strongly influenced by the degree of hydration and nanoscale ordering within the membrane. Density-hydration relationships in Nafion have been probed experimentally and computationally for decades. In this work, we examine how local structure determine the density properties, which allows us to interpret experimental observations and results from models, as well as their deviations from theoretical predictions. We observed changes in water phase morphology not only on hydration levels, but on structural configurations as well, we have considered amorphous and crystalline systems. Well hydrated membrane, which ensure connected water domains is crucial for fuel cell performance, enabling a pathway for proton transport. Water clustering in Nafion membranes was analyzed using the DBSCAN algorithm, which groups closely packed molecules while distinguishing sparse regions as noise. This approach enabled the identification of arbitrarily shaped water aggregates and reduced the influence of outliers. The analysis revealed a clear structural transition with hydration: at low water content, water molecules form small, isolated clusters with limited connectivity; at moderate hydration, larger clusters emerge and begin to percolate in crystalline systems; and at high hydration, nearly continuous water networks develop, spanning the entire simulation domain. Additionally, we determined how water content

and membrane structure influence the density of the hydrated Nafion membrane. For all levels of hydration, crystalline configurations have higher densities compared to their amorphous counterparts. That occurs because the spatial ordering allows hydrophobic Nafion backbones to pack closely together with water channels following the direction of the backbones. On the other hand, the globulated nature of the water channels in the amorphous configurations hinders the packing of the backbones, resulting in lower density. Voronoi tesselation analysis reveal that crystallinity enhances molecular packing, yielding higher effective density of the polymer matrix compared to the less ordered amorphous structures. Overall, our findings provide a deeper understanding of how structural ordering influences the density, hydration, and mechanical properties of polymer systems. The interplay between crystallinity and hydration has broad implications for the design of functional polymer materials, particularly in applications such as fuel cell membranes, hydrogels, and biomimetic systems. A combination of molecular simulations, structural analysis, and theoretical modeling offers a powerful framework for predicting the material behavior in hydrated environments, hence guiding future experimental and computational studies in this scientific field.

Serbian Ceramic Society Conference
ADVANCED CERAMICS AND APPLICATION XIII
New Frontiers in Multifunctional Material Science and Processing

Serbian Ceramic Society
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PROGRAM AND THE BOOK OF ABSTRACTS

Hotel Zira, Ruzveltova 35
Serbia, Belgrade, 8-10th September 2025.

Conference Topics

- Basic Ceramic Science & Sintering
- Nano-, Opto- & Bio-ceramics
- Modeling & Simulation
- Glass and Electro Ceramics
- Electrochemistry & Catalysis
- Refractory, Cements & Clays
- Renewable Energy & Composites
- Amorphous & Magnetic Ceramics
- Heritage, Art & Design

Conference Programme Chairs:

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P4

Comparison of Interactions and Morphology During Aluminum Fluoride and Water Intercalation in Graphite

Sindy J. Rodríguez[1], Mateja Jovanović[2,3], Miljan Dašić[4], Igor Stanković[4,5]

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Understanding the intercalation behavior of ionic and molecular species in graphite is essential for advancing layered and two-dimensional material applications. In this study, we present a comparative investigation of the structural, energetic, and morphological features associated with the intercalation of aluminum fluoride (AlF_3) and water molecules into graphite. By combining molecular dynamics simulations with density functional theory calculations, we evaluate interlayer spacing, binding energies, and interaction mechanisms of both intercalants within the graphite host. The results reveal distinct intercalation pathways and interfacial morphologies: water molecules induce interlayer swelling and exhibit a homogeneous distribution between graphene sheets, while AlF_3 forms rigid, localized domains stabilized primarily by electrostatic interactions. These contrasting behaviors lead to markedly different structural responses in the graphite matrix. The insights gained from this comparative study offer valuable guidance for the design of graphite-based materials tailored for electrochemical devices and layered composite systems.

We acknowledge funding from the European Union's Horizon Europe research and innovation program under the Marie Sklodowska-Curie project BLESSED grant agreement No-101072578.

European Biophysics Journal (2025) 54 (Suppl 1):S1–S273
https://doi.org/10.1007/s00249-025-01757-9

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This supplement was not sponsored by outside commercial interests.
It was funded entirely by the publisher.

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Inspection of snapshots from a previously reported QM/MM MD simulation of the reactants state region provided two interesting observations: i) An ester bond between formate and nicotinamide spontaneously formed and subsequently dissociated. Such an ester bond was earlier predicted to form with negligible energy barrier in gas phase but was not yet reported in QM/MM MD simulations. ii) Two snapshots were identified as possible near-attack conformations (NACs) from which the transition state (TS) can be reached by unhindered rotation of formate about its O-O axis. The two NACs differ from each other in the direction of rotation required to attain the TS. Calculation of natural orbitals for chemical valence (NOCV) channels indicated genesis of the new C-H bond already at the NAC stage. Importantly, both NACs feature a nonlinear C(formate)-H(formate)-C(nicotinamide) angle, approaching linearity only in the TS. We believe that due to the particular conception of the active site which profits from the unique triangular shape of formate, the formate-nicotinamide couple can reach the TS more easily through the rotational movement of formate than through its parallel shift along the C-H vector, the pathway advocated so far. Supported by e-INFRA CZ project, MetaCentrum and CERIT-SC.

P-3.20

Induced Conformational Opening of Switch I In Gtp-bound Ran Gtpase

Janka Czigleczki [1], Balint Dudas [2], Erika Balog [1]
[1] Semmelweis Univeristy, Budapest, Hungary
[2] National Institutes of Health, Bethesda, MD, United States

Ran is a key regulator of nucleocytoplasmic transport through the nuclear pore complex. As other small GTPases, Ran functions as a molecular switch, cycling between an inactive GDP-bound state and an active GTP-bound state. Structurally, Ran it is composed of a globular G-domain and a C-terminal region, that includes a C-terminal helix. The functional elements switch I and switch II of the G-domain undergo major conformational changes upon the GTP/GDP exchange, with switch I shifting from a closed to an open conformation. This conformational regulates the binding of downstream partners. Here, we describe an induced conformational transition of RanGTP switch I from the closed 'on' conformation to an open 'off' conformation resembling that of RanGDP obtained by MD simulations. Our findings indicate that the opening of switch I occurs consistently when the interaction within the triad comprising Phe35-GTP-Lys152 is permanently disrupted, specifically due to the reorientation of Lys152. Our results could have broader implications in for drug development targeting small GTPases containing point mutations that lock switch I in the closed 'on' conformation, potentially leading to uncontrolled cell proliferation in various cancers.

P-3.21

The Role of Allosteric Effects in the Crm1-rangtp Complex Formation

Janka Czigleczki [1], Hyunbum Jang [2], Ruth Nussinov [2], Erika Balog [1]
[1] Department of Biophysics and Radiation Biology, Semmelweis University, Budapest, Hungary
[2] Computational Structural Biology Section, Frederick National Laboratory for Cancer Research in the Cancer Innovation Laboratory, NCI, Frederick, MD, United States

Small GTPase Ran (Ras-related Nuclear protein) is the main regulator of the nucleo-cytoplasmic transport through the nuclear pore complex. It functions as a molecular switch cycling between the GDP-bound inactive, "off" and GTP-bound active, "on" state. Since deregulation of Ran is linked to numerous cancers, understanding the complexity of its regulatory mechanism, is critical for drug discovery. One of the partners in the nucleo-cytoplasmic transport is the export receptor CRM1 (chromosome region maintenance 1). CRM1 cooperatively binds RanGTP and cargo in the nucleus. In the transport complex, RanGTP is localized within the ring-like structure of CRM1. In the crystal structures of the CRM1-RanGTP, the structure of the Ran C-terminal segment remains unresolved. Using MD simulations, our goal was to uncover the molecular mechanisms that starts form the CRM1-RanGTP binding and leads to the closed macromolecular complex.

P-3.22

Multi-scale Modeling of Enzyme-substrate Interactions in Crowded Environments

Miljan Dašic [1], Ashwathi Poolamanna [1], Mehrnoosh Khodam Hazrati [1], Štepán Timr [1]
[1] J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences, Prague, Czech Republic

Formation of enzyme assemblies and substrate channeling have been suggested as key factors controlling metabolic efficiency, yet the role of crowded cellular environments in these processes remains insufficiently understood. We present a multi-scale modeling approach that integrates coarse-grained (lower spatio-temporal scales) with reaction-diffusion (higher spatio-temporal scales) simulations via Markov state model analysis. The coarse-grained molecular simulations describe the local environment within enzyme assemblies as well as the interactions among enzymes, substrates, and crowders. Trajectories generated by these simulations enable the determination of kinetic parameters by applying Markov state model analysis. This analysis reveals how interactions in the crowded environment affect the kinetics of substrate transitions between distinct binding states. Moreover, the information gained about the kinetics of the system serves for the derivation of parameters needed for the construction of stochastic reaction-diffusion simulations, which allow the investigation of processes in large-scale enzyme assemblies. Our work provides insights into the impact of inert and attractive crowders on substrate diffusion, binding to enzymes, and ultimately, the efficiency of metabolic pathways.

P-3.23

A Machine Learning Approach to Identify Carbon Dioxide Binding Proteins for Sustainability and Health

George Weston [1], Matteo Degiacomi [2], Martin Cann [1]

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[2] University of Edinburgh, Edinburgh, United Kingdom

Carbon dioxide (CO2) has a fundamental role in biological processes throughout the biosphere. While much is known about the impact of CO2 on the overall physiology of an organism, much less is known about how its interaction with specific biomolecules may affect their function [1, 2]. Our work focusses on carbamylation, a non-enzymatic reversible protein post-translational modification (PTM) where CO2 binds onto the neutral lysine ε-amino groups [3]. A novel mass spectrometry-based experimental technique, TEO trapping, has been recently used to demonstrate that, for reasons yet unclear, CO2 does not bind to every lysine [2]. While informative, this experimental technique is laborious, which limits our ability to gain a clear and comprehensive view of the interactions between CO2 and proteins. For this reason, we are carrying out extensive molecular dynamics simulations and developing a computational method to predict which lysine, in any protein, may undergo carbamylation. We found that standard metrics (pKa, solvent accessible surface area, and amino acid depth) are insufficient to singlehandedly explain why some lysine may be modified, but not others. Therefore, we are now exploring the usage of atomic environment vectors, commonly used in machine learning, for this classification task.

P-3.24

Computer Simulations of the Bacterial Ribosome Using a General Purpose Coarse-grained Model Martini

Michal Kolar [1], Josef Cikhart [1]
[1] University of Chemistry and Technology, Prague, Czech Republic

Ribosomes are critical biomolecular nanomachines responsible for protein synthesis in all known organisms. The function and dynamics of ribosomes can be studied using molecular dynamics computer simulations. Although this task remains challenging at atomic level, several studies have reported all-atom molecular dynamics simulations of the entire ribosome. However, for certain applications, atomistic simulations are impractical due to the limited simulation timescales achievable. In this study, we investigate the applicability of the coarse-grained MARTINI model for simulations of the bacterial ribosome. After testing several simulation setups, we found that the structure of the ribosome and its components are generally well represented compared to the reference experimental structure. Compared with all-atom simulations of the entire ribosome, coarse-grained simulations result in a less flexible and smaller ribosome. We demonstrate how modifications of some parameters of the model can enhance the dynamics of the ribosome to better align with the atomistic model. Our work provides a detailed protocol for coarse-grained simulations of the ribosome and highlights aspects of the model that need improvements.

P-3.25

Substrate and Cofactor Binding in Sult1a1 Dimer Governed by Allosteric Mechanisms

Daniel Toth [1], Balint Dudas [2], Arnaud B. Nicot [3], Maria A. Miteva [4], Erika Balog [1]
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[2] Laboratory of Computational Biology, National Heart, Lung, and Blood Institute, National Institutes of Health, Bethesda, MD 20892, Bethesda, MD 20892, United States
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[4] Université Paris Cité, CiTCoM UMR 8038 CNRS, INSERM U1268 MCTR, Paris, France

Sulfotransferases (SULTs) are a class of phase II drug-metabolizing enzymes that play a crucial role in the metabolic processing of a wide range of endogenous and xenobiotic compounds. SULTs form homodimers in vivo. Since it has been shown that the monomers of SULT1A1 isoform maintain their activity in vitro, the biological significance of dimerization remains unclear. However, experimental results show that dimers exhibit greater catalytic efficiency and stability. To elucidate the mechanism and the effects of dimerization, molecular dynamics (MD) simulations were conducted on the monomer and dimer form of the enzyme, containing no ligands (apoenzyme), cofactor, and cofactor+substrate. Furthermore, force distribution analysis (FDA) was used to investigate the dynamic effect of cofactor and substrate binding on the dimer structure. The obtained results demonstrate a clear effect on the apo-dimer on the increase of the ligand binding gate opening and greater fluctuation of the functional loops of one monomeric subunit. Furthermore, in the dimer, both intra- and inter-subunit allosteric effects have been identified as a direct consequence of cofactor and the substrate binding.

P-3.26

Substrate Binding in Enzyme Clusters: Effects of Crowders and Transient Interactions

Ashwathi Poolamanna [1], Miljan Dašic [1], Mehrnoosh Khodam Hazrati [1], Štepán Timr [1]
[1] J. Heyrovsky Institute of Physical Chemistry, Praha 8, Czech Republic

In living cells, various enzymes have been found to assemble into transient structures that can appear and disassemble depending on external conditions. Such assemblies have been found in various pathways, including glycolysis, oxidative phosphorylation, purine synthesis, etc. However, the molecular mechanisms driving their formation and functional relevance remain poorly characterized.
In this study, we develop a highly coarse-grained computational model based on insights from all-atom molecular dynamics simulations to investigate how the presence of crowders as well as transient interactions between enzyme assembly constituents—enzymes,

MecaNano General Meeting 2025

19-21 May 2025 Krakow (Poland)

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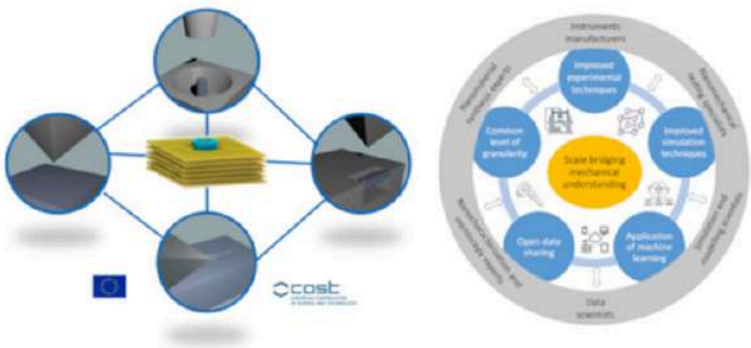
General Meeting of MecaNano COST Action 2025

MecaNano stands for "European Network for the Mechanics of Matter at the Nano-Scale" is a European Cooperation in Science & Technology (COST) Action running 2022-2026. The Action is intended as a broad international cooperation aiming to advance the multiscale understanding of the mechanical behavior of nanostructured materials. By combining the expertise of its participants – from experimentalists to simulation, data management and machine learning experts – it aims to overcome the different bottlenecks limiting the exploration of mechanical size effects. MecaNano provides its members with numerous opportunities to interact and collaborate, e.g. through dedicated workshops, symposia and summer schools, or by funding the mobility between participants.

This **Third General Meeting** will bring together all stakeholders of the MecaNano community in order to discuss scientific progress in our field(s) and plan common activities. We are looking forward to your participation! This meeting is a good opportunity to meet your counterparts of the small-scale mechanical characterization community.

We do not charge a conference fee but you must register on this website in time before the meeting. **Submitting an abstract is not registering.**



The General Meeting is opened to oral and poster contributions related to all topics covered by MecaNano:

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- Experimental and simulation investigations, including
  - Nanoindentation
  - Nanomechanical testing
  - Advanced characterization methods
  - Atomistic and Meso-scale simulations
  - Finite elements
  - Crystalline, amorphous or hybrid materials
- Management of research data in materials science
- Machine learning applications related to the topics above

Regular presentations will be 20 min long including Q&A. Poster size is A0 (portrait orientation is preferred). Please provide an abstract of max. 250 words **until 14. February 2025**.
Let's connect together!

MecaNano
COST Action CA21121

Poster list		
Poster session: Tuesday 16:50		
1	Mohammed Tahir Abba	Toward High Strain Rate Spherical Nanoindentation Testing
2	Fabien Amiot	Second strain-gradient elasticity for centro-symmetric cubic materials
3	Muhammet Anıl Kaya	Mechanical Characterization of Hazelnut Shell Powder-Reinforced Epoxy Composites for Sustainable Applications
4	Tizian Arold	Nitrogen-Doped PVD MoS2 Coatings: Enhanced Wear Resistance and Tribological Performance in Rolling-Sliding Contact
5	Saulius Baskutis	Investigation of the Potential of PTFE Coatings for Journal Bearings
6	Samuel Bojarski	High-strength and non-brittle crystalline-amorphous PVD-ALD nanolaminates of amorphous alumina and AlCoCrFeNi high-entropy alloy
7	Jaroslav Cech	Nanoindentation study of NiTi shape memory alloys
8	Grzegorz Cios	Orienting grains for nanomechanical testing without EBSD
9	Özgen Ümit Çolak Çakır	Machine Learning in Thermoset Polymer Creep Modeling
10	Diego Cruañes	Understanding nanoindentation statistical dispersion in ceramic - metal cemented carbides by numerical simulation and FIB tomography
11	Arjun Bharath Curam	Defect-driven microstructural evolution and mechanical characterization of CoCrNi, Fex(CoCrNi)100-x and CoCrNi/Fe nanolaminate complex compositional alloy thin films
12	Miljan Dašić	Selecting Protein Crystal Structure for Optimal Scoring of Protein-Ligand Interactions
13	Emine Özlem Dengiz	Investigation of the Mechanical Behavior of Graphene-Reinforced Magnesium via Experimental and Finite Element Method
14	Cengiz Görkem Dengiz	Investigation of the Mechanical Behavior of Graphene-Reinforced Magnesium via Experimental and Finite Element Method
15	Oğuzhan Der	Quantitative Analysis of Nanoscale Mechanical Behavior in Hybrid Materials Through Nanoindentation and FEM Simulations
16	Francisco Javier Dominguez–Gutierrez	Nanoindentation and Defect Dynamics in Irradiated Fcc NiFe Alloys: Insights from Experiments and Atomistic Modeling
17	Marco Ezequiel	Suppressing shear band instability for strong and ductile crystal/glass nanolaminates
18	Lala Gahramanli	Analysis of the physical properties of CdxZn1-xS-based nanocomposites synthesized through sonochemical and SILAR methods
19	Julien Guénolé	Interfaces as dislocation density fields for bridging length scales in nanomechanics
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21	Evghenii Harea	Comparative Analysis of the Gao-Nix Model and Multifractal Scaling Law Model for Indentation Size Effect
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23	Benedykt Jany	Integrating Machine Learning and Data Mining Techniques with Surface Texture Analysis to Explore Wetting and Optical Properties of CuAg Alloys
24	Piotr Jenczyk	Modification of the matrix-reinforcement interface in Ni-SiC composites

Selecting Protein Crystal Structure for Optimal Scoring of Protein-Ligand Interactions

Miljan Dašić*†[1,2], Jindřich Fanfrlík[1], and Jan Řezáč[1]

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[2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade – Serbia

Abstract

Non-Covalent Interactions between target protein (P) and ligands (L) determine the P-L binding affinity. Appropriate approach for modeling P-L binding is based on Semi-empirical Quantum-Mechanical (SQM) methods. Promising solution for determining P-L binding affinity predictions is universal physics-based scoring function SQM2.20. Term predictions refers to the fact that results obtained via simulations are confronted with reliable experimental results. Performance of SQM2.20 has been rigorously verified over a benchmark dataset named PL-REX (Protein–Ligand Refined EXperiment) consisting of high-resolution crystal structures and reliable experimentally determined P-L binding affinities (PL-REX comprises 10 diverse protein targets, with 164 QM-optimized P-L complexes).

We have examined the variability of SQM2.20 scoring using a single receptor, in case of each protein target of PL-REX. System preparation for scoring includes annealing of hydrogen atoms in protein. Hydrogen annealing is affected by the value of random seed, which is set as input parameter. Out of 100 considered cases (10 protein targets x 10 different random seeds), 94 cases belong to the interval with absolute difference in squared Pearson coefficient R^2 from the value averaged per protein target of 0.05. Such result allowed us to establish the difference in R^2 values of $2 \cdot 0.05 = 0.1$ as a significant change in scoring results.

Each of protein targets of PL-REX comprises different protein crystal geometries. The same applies to protein crystal geometries of two additional CDK2 systems, which were considered. We have investigated the impact of protein crystal structure on SQM2.20 scoring result over PL-REX dataset and two additional CDK2 systems in the next two cases: within ligand series, and when using protein crystals with different ligands (here CDK2 protein target was used as an example). Our general conclusion is that the sensitivity of scoring on crystal's geometry is low, which is advantageous for applications.

*Speaker

†Corresponding author: mdasic@ipb.ac.rs

Regensburg 2025 – scientific programme

CPP: Fachverband Chemische Physik und Polymerphysik

CPP 23: Polymer and Molecular Dynamics, Friction and Rheology

CPP 23.5: Talk

Wednesday, March 19, 2025, 10:45–11:00, H34

selection status for this contribution: according to the sessions' setting

Role of Trapped Water Molecules at Sliding Contacts in Lattice-Resolved Friction Investigated with Molecular Dynamics — •Miljan Dašić and Igor Stanković — Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Understanding nanoscale friction within an environment which contains water, is crucial for engineering friction-based mechanisms and characterizing surfaces. From the point of view of Friction Force Microscopy (FFM) experiments, it has been understood that the lattice resolution in water environments originates from a dry contact state, in case of which all water molecules get expelled from the gap between the microscope's tip and the studied substrate.

We have developed an All-Atom Molecular Dynamics simulation setup, for revisiting this understanding by performing a detailed analysis of the impact of water molecules present in the system on the dynamic behavior of the nanotribological contact between an amorphous SiO2 probe and a monolayer MoS2 substrate.

Our analysis of stick-slip patterns shows the entrapment of water molecules at the contact interface. These trapped water molecules act as an integral part of the probe and participate in its interaction with the substrate, hence affecting the probe's dynamics and preventing long slips. Surrounding water molecules from the capillary or layer of water exhibit a replenishing effect, acting as a water reservoir during the sliding process. Such a phenomenon enables the preservation of lattice-scale resolution across a range of normal loads.

Keywords: Molecular Dynamics; Molybdenum Disulfide; Water; Friction; Stick-Slip

Regensburg 2025 – scientific programme

CPP: Professional Association for Chemical Physics and Polymer Physics

CPP 15: Poster Session I

CPP 15.30: Poster

Monday, March 17, 2025, 19:00–21:00, P4

selection status for this contribution: according to the sessions' setting

Evaluating the Properties of Nafion PEMFC Membrane via MD Simulations — •Mateja Jovanovic[1], Matthias Baldofski[1], Igor Stankovic[2], Marcin Rybicki[1], and Miljan Dašić[2] — [1]Freudenberg Technology Innovation SE & Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Understanding the nanoscale interactions within Nafion membranes is crucial for optimizing their performance in Proton Exchange Membrane Fuel Cells (PEMFC). In present a molecular dynamics study of the structural and dynamic properties of Nafion-water systems under varying hydration levels using molecular dynamics simulations. The density of the Nafion-water system is examined to identify deviations from the ideal additivity rule, providing insights into molecular interactions and structural rearrangements. The radial pair distribution function, radius of gyration, pore-water contact surface, and diffusion coefficients for water and hydronium ions are analyzed to reveal the local organization, solvation quality, porosity, and transport properties within the hydrated Nafion membrane. The methodology used to obtain properties of the Nafion-water mixture builds on techniques previously developed for the study of ionic liquids [1].

[1] I. Stanković, M. Dašić, M. Jovanović, A. Martini, Langmuir 2024, 40(17), 9049-9058, doi:10.1021/acs.langmuir.4c00372

Keywords: Molecular dynamics; PEMFC; Nafion membrane; Transport properties

CERTIFICATE

We hereby certify that

Miljan Dašić
(CTU Prague & Institute of Physics Belgrade)

has attended the 11th International Conference on Multiscale Materials Modeling, held in Prague, Czech Republic from September 22 to 27, 2024.

Contribution

Talk, presented: 24/09/2024 04:10 PM
Integrating Newton's Equations of Motion in the Reciprocal Space as a Novel Materials Modeling Technique
Poster, presented: 24/09/2024 05:20 PM
Reactive Molecular Dynamics Study of the Nanotribological Properties of Oxidized

Roman Gröger
Conference Chair
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Session Program – Tuesday, 24 September

Room: Chamber Hall

09:50 AM	10:20 AM	**Coffee break**	Forum Hall Foyer 2
		Symposium H - Tuesday Morning / 10:20 AM-12:10 PM	Chair: Takeshi Egami
10:20 AM	**10:50 AM**	**Keynote Lecture: A model of thermodynamic stabilization of nanocrystalline grain boundaries in alloy systems**	**Yuri Mishin**
10:50 AM	11:10 AM	Multiscale model predicting brittle fracture of nanocomponents	Miroslav Černý
11:10 AM	11:30 AM	The Energetics of Disconnection Nucleation and Glide in Symmetric Tilt Grain Boundaries	Himanshu Joshi
11:30 AM	11:50 AM	Capabilities and improvement ability of classical many-body potentials: application to hcp-Zr	Alessandra Del Masto
11:50 AM	12:10 PM	Insights into Shear-Coupled Twin Boundary Migration: A Comprehensive Analysis	Ritu Verma
12:10 PM	01:10 PM	**Lunch**	Forum Hall Foyer 2
		Symposium H - Tuesday Afternoon / 01:10 PM-03:00 PM	Chair: Yuri Mishin
01:10 PM	**01:40 PM**	**Keynote Lecture: Atomistic simulations in multi-principal-component FCC materials**	**Diana Farkas**
01:40 PM	02:00 PM	Phase Pattern Formation in Grain Boundaries	Ian Winter
02:00 PM	02:20 PM	Revealing and Controlling of Dislocation Plasticity, Twinning and Fracture in BCC Transition Metals and Alloys	Zhaoxuan Wu
02:20 PM	02:40 PM	Investigation of Impacts of Spin Inhomogeneity on Screw Dislocation Mobility in BCC Iron	Hideki Mori
02:40 PM	03:00 PM	Revisiting Franks Theory for the creation of open-core screw dislocations in 4H-SiC by molecular dynamics simulation	Georg Holub
03:00 PM	03:30 PM	**Coffee break**	Forum Hall Foyer 2
		Symposium H - Tuesday Afternoon / 03:30 PM-05:20 PM	Chair: Diana Farkas
03:30 PM	**03:50 PM**	**Atomistic Mechanisms of Ring Formation During Catalyzed Carbon Nanotube Growth**	**Wang Rui**
03:50 PM	04:10 PM	Relating Shear Transformations in a Model Glass to Features of the Two-Dimensional Local Yield Surface	Spencer Fajardo
04:10 PM	04:30 PM	Integrating Newton's Equations of Motion in the Reciprocal Space as a Novel Materials Modeling Technique	Miljan Dašić
04:30 PM	04:50 PM	Pseudo-twin boundary improves flow stress and fatigue resistance of TiAl single crystal: atomistic simulations	Prof. Dr. Min Yi
04:50 PM	05:10 PM	-	-
05:20 PM	**07:20 PM**	**Poster Session 1**	**Forum Hall Foyer 3**
07:20 PM	**07:40 PM**	**Poster Award Ceremony**	**Chamber Hall**

Poster session 1

Tuesday - September 24, 2024

17:20-19:20 Forum Hall Foyer 3

Sy	Partic	Presenter	Title
A	3234	Dmitry Bachurin	DFT study of helium dynamics in titanium beryllides
A	3310	Fraser Birks	QM/MM Style Potential Coupling to Accelerate Simulations
A	3252	Hyejeong Song	Theoretical investigation for kinetically pumped charge multiplication in colloidal quantum dots
A	3238	José David Cremé Angel Bello	A DFT model of the W(110)/Cu(111) interface
A	3357	Reyhaneh Ghassemizadeh	Stability and electronic structure of NV centers at dislocation cores in diamond
A	3031	Yosvany Silva Solís	Diffusion modelling of H isotopes through the W/Cu interface
A	3566	Zixiong Wei	Oxygen adsorption behavior on various BCC Fe surfaces: A Density Functional Theory study
A	3570	Martin Friák	Combined theoretical and experimental study of Fe-Sn intermetallic phases
A	3773	Haneul Kim	Catalytic performance of Ru- and W-doped ZrO2 and CeO2 for H2O2-based scavenger reactions: NEB-DFT investigations
A	3778	Ahmed Gueddouh	DFT investigation of the extraordinary properties of the machinable layered ternary nitrideW2AlN
B	3535	Amine Benzerga	A discrete dislocation plasticity analysis of size effects in torsion
B	3199	Balduin Katzer	A graph database for feature characterization of dislocation networks
B	3458	Dan Mordehai	Stochastic strain-to-failure of twinned nanowires
B	3099	Laurent Pizzagalli	Plastic deformation in nano-objects: relation between applied stress and local stresses as a function of size and shape
B	3194	Ronan Madec	A semi analytical approach for slip system interactions
B	3192	Rong Mu	Constructing high-density dislocations by primary (Nb,Ti)(C,N) to induce massive secondary precipitations in austenitic heat-resistant cast steel during long-term aging
B	3504	Ryan Sills	Strength and formation rates of junctions in FCC metals
B	3195	Shuhao Ren	Microstructure Evolution, Strengthening Mechanism, and Fatigue Wear Behavior of Hot Rolled Wear-resistant Steel
B	3241	Vasily Bulatov	Dislocation locks are all distructible
B	3247	Yang Li	A multiphysics framework for defects evolution at the mesoscale
B	3008	Yves-Patrick Pellegrini	Dynamic Shock-Driven Dislocation Dipole Nucleations In a Peierls Model
C	3124	Baptiste Bienvenu	Anomalous slip in body-centred cubic metals
C	3302	Jonathan Amodeo	Pyrough : a new tool to model sample roughness in atomistic and finite element simulations
C	3058	Markus Stricker	Mesoscale modeling of grain boundaries: a model for physical transmission of dislocations through grain boundaries
C	3222	Matthew Maron	High-Temperature Compression of Zr and Refractory HEA Micropillars: Modelling and In-Situ Experiments
C	3563	Rui Wang	Developing Extended Modified Embedded-Atom Method Potentials for Atomistic Modelling on Plastic Deformation of BCC Transition Metals
C	3185	Sing-Huei Lee	A data-based derivation of the internal stress in the discrete-continuum transition regime for dislocation-based plasticity
C	3717	Sweta Kumari	Revisiting the statistics of incipient plasticity
C	3210	Tomotsugu Shimokawa	Interface mediated plasticity in hetero-nanostructured Ti through atomic simulation
C	3742	Berkin Bal	Determination of Cold Work Amount by Mechanical Spectroscopy
E	3660	Anirvinya Samanyu Tirumala	An empirical potential for simulating the effects of helium and hydrogen isotopes in highly irradiated tungsten
E	3506	Anter El-Azab	Dynamics of Discrete Defect Clusters in Irradiated Solids
E	3303	Arnaud Allera	Efficient structural analysis using atomic descriptors
E	3500	Cristian D. Denton Zanello	Creation of a helical structure in a screw dislocation in FeCr and Fe due to the presence of close collision cascades.
E	3697	David Cereceda	A first-principles study on the structural-thermodynamics properties of tungsten-based plasma-facing materials
E	3154	Duc Nguyen-Manh	Multi-scale modelling of detritiation in tungsten and its oxides
E	3061	Enrique Martinez	From anti-Arrhenius to Arrhenius behavior in a dislocation-obstacle bypass: Atomistic simulations and theoretical investigation
E	3656	Faith Kporha	Sputtering of tungsten and deuterium decorated tungsten surfaces
E	3086	Jean-Paul Crocombette	Energy stored by defects in CaWO4 ultra low temperature bolometers calculated from cascade simulations with machine learning potentials.
E	3333	Amil Aligayev	Evolution of Vacancy Defects in Ni-Based Concentrated Solid-Solution Alloys Driven by Collision Cascades
E	3322	Jan Wróbel	Combined effects of irradiation and C/N interstitials in Fe – 3.28 at. % Cr alloys
E	3374	Pamela Camilos	Atomic-scale modeling of diffusion in concentrated alloys
E	3632	Sara Adibi	Unraveling Time-Temperature Superposition in Cavitation Resistance of Metals with Nonequilibrium Vacancy Concentrations
E	3708	Elchin Huseynov	Metal-semiconductor transition investigation of nanocrystalline silicon carbide under neutron irradiation
E	3118	Thomas Jarrin	Multiscale simulation of atomic displacements in semiconducting materials
E	3097	Inam Iqbal Lalani	Mechanisms of shear localization in high-temperature BCC micropillar compression
H	3002	Andrej Ostapovec	Some aspects of (1 1 -2 2) twinning in hcp metals
H	3260	Anissa Acheche	Thermal stability of High Entropy Alloy Nanoparticles: an atomic scale study
H	3276	Jae Hur	Atomistic investigation of phase transformations in NiTiCu shape memory alloys
H	3227	Jea-Young Hwang	Molecular dynamics simulation study on the deformation behavior of nanotwined NiMo alloys
H	3018	Kaito Saito	Finite-Temperature Molecular Dynamics Simulation of BCC Iron Grain Boundary Fracture Using Machine Learning Potentials.
H	3263	Lei Zhang	Developing machine learning potentials for modeling cracks and dislocations in bcc iron
H	3650	Miljan Dašić	Reactive Molecular Dynamics Study of the Nanotribological Properties of Oxidized Vanadium
H	3484	Santhosh Mathesan	Dislocation microstructure informed topology in Nanoporous Au Nanopillars
H	3169	Margot Lucas	On the Stability of Nanovoids in Fcc Metals and the Influence of Hydrogen

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Comparison of properties of phosphonium ionic liquids mixed with water

Mateja Jovanović[1,2], Igor Stanković[3], and Miljan Dašić[3,4]

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[2] *Freudenberg Technology Innovation SE & Co. KG, Weinheim, Germany*
[3] *Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Zemun, Serbia*
[4] *Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic*

Author list: **Mateja Jovanović**, Igor Stanković, Miljan Dašić

We present a numerical investigation of the influence of water content on the dynamic properties of a family of phosphonium-based room-temperature ionic liquids. The study presents a compelling correlation between structural changes in water−ionic liquid solutions and thermodynamic and transport properties across diverse systems. The results for phosphonium ionic liquids are compared with 1-butyl-3-methylimidazolium hexaphosphate ([bmim]PF_6) as a reference. Through this approach, phosphonium cation structure-related characteristics can be identified and placed within the broader context of ionic liquids. These insights are underpinned by observed changes in interaction energy, boiling point, diffusion rate, and viscosity, highlighting the crucial role of water molecules in weakening the strength of interactions between ions within the ionic liquid. The investigation also explains temperature-dependent trends in phosphonium cations, showing that alkyl group length and molecular symmetry are important tuning parameters for the strength of Coulomb interactions. These results contribute to a refined understanding of phosphonium ionic liquid behavior in the presence of water, offering valuable insights for optimizing their use in diverse fields.

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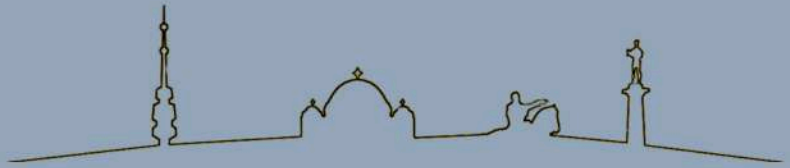

3rd International Conference on Noncovalent Interactions, 2024, Belgrade

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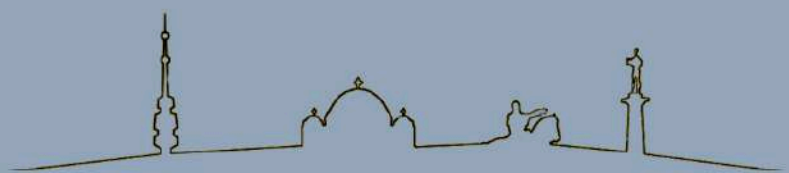

Sensitivity of the Scoring of Protein-Ligand Binding Affinity Predictions on Protein Crystal's Geometry

Miljan Dašić,[1] Jindřich Fanfrlík[1], and Jan Řezáč[1]

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Keywords: Protein-Ligand binding affinity predictions; PL-REX benchmark dataset; semiempirical quantum-mechanical methods; physics-based scoring function SQM2.20; impact of crystal's geometry

Noncovalent Interactions (NCI) between a target protein and ligands determine the P-L binding affinity. Appropriate approach for modeling the P-L binding is based on the Semi-empirical Quantum-Mechanical (SQM) methods. Those methods are quantum-mechanical in the core, but they also include the semi-empirical corrections of the NCI.

Accurate and fast determination of Protein-Ligand (P-L) binding affinity predictions is highly relevant for the Structure-Based Drug Design (SBDD) branch of the Computer-Aided Drug Design (CADD) discipline. Naturally, an efficient solution of this problem would be very attractive regarding the possible applications in pharmaceutical drug discovery/design, e.g., in hit identification and lead optimization.

A promising solution for determining the P-L binding affinity predictions is an universal physics-based scoring function SQM2.20[1]. Its performance has been rigorously verified over a benchmark dataset PL-REX[1] consisting of high-resolution crystal structures and trustworthy experimentally determined P-L binding affinities (PL-REX consists of 10 diverse protein targets, with 164 QM-optimized P-L complexes).

Each of the ten protein targets of the PL-REX dataset includes different protein crystal geometries. We have investigated the sensitivity of the scoring on crystal's geometry. Besides that, for each protein target we have determined the best reference crystal, i.e., that crystal which maximizes the scoring results.

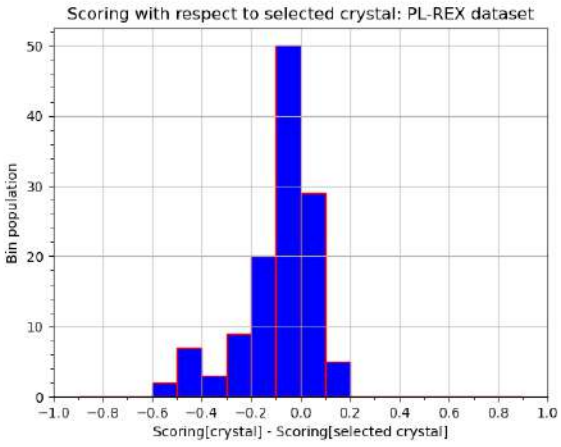

Table 1. Overview of the scoring results (Pearson R^2) for the PL-REX dataset

References

[1] Pecina, A.; Fanfrlík, J., Lepšík, M., Řezáč, J., Nature Communications **2024**, *15*, 1127.

MAIN MENU

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GENERAL MEETING OF MECANANO COST ACTION 2024

MecaNano stands for "European Network for the Mechanics of Matter at the Nano-Scale" is a European Cooperation in Science & Technology (COST) Action running 2022-2026. The Action is intended as a broad international cooperation aiming to advance the multiscale understanding of the mechanical behavior of nanostructured materials. By combining the expertise of its participants – from experimentalists to simulation, data management and machine learning experts – it aims to overcome the different bottlenecks limiting the exploration of mechanical size effects. MecaNano provides its members with numerous opportunities to interact and collaborate, e.g. through dedicated workshops, symposia and summer schools, or by funding the mobility between participants.

This **Second General Meeting** will bring together all stakeholders of the MecaNano community in order to discuss scientific progress in our field(s) and plan common activities. We are looking forward to your participation! This meeting is a good opportunity to meet your counterparts of the small-scale mechanical characterization community.

Final Program is available!

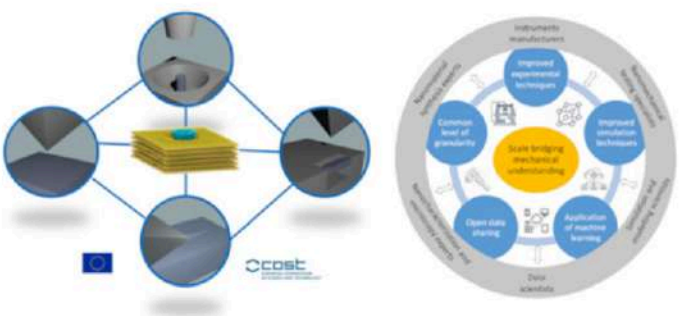
Final Program and Abstract Book

Final Program

Please note: Poster printing is not available by the event organizers. If you believe you will have troubles transporting a poster please contact the organizers and you may send the **printed poster** to the local organizers ahead of the meeting. Otherwise, you can use the internet to find a suitable printer around TU Wien to print your poster. Another option is "Poster Smith" and they can print on fabric.

Poster size is A0 (portrait orientation is preferred). There is no MecaNano specific template for posters. Poster Presenters are free to use any template.

We do not charge a conference fee but you must register on this website in time before the meeting. **Submitting an abstract is not registering.**



Call for abstracts is closed

The General Meeting is opened to oral and poster contributions related to all topics covered by MecaNano:

- Mechanical size effects and nanoscale deformation mechanisms
- Experimental and simulation investigations, including
  - Nanoindentation
  - Nanomechanical testing
  - Advanced characterization methods
  - Atomistic and Meso-scale simulations
  - Finite elements
  - Crystalline, amorphous or hybrid materials
- Management of research data in materials science
- Machine learning applications related to the topics above

Regular presentations will be 20 min long including Q&A. Poster size is A0 (portrait orientation is preferred).

Please provide an abstract of max. 250 words **until 5. March 2024.**

Let's connect together!

14:30	COFFEE BREAK	
SESSION 4: Machine learning and mechanical behavior *Chair: Claus Trost*		
15:00	Peter Isprovity (Invited)	Deciphering acoustic emission using micromechanical experiments
15:30	Krzysztof Wieczerzak	Exploring CuAgZr metallic glasses for biomedical use: A study using combinatorial synthesis, high-throughput experiments, and machine learning
15:50	Stanislav Zak	Thin film nanoindentation and the importance of the tip radius
16:10	Michael Wurmshuber	Micromechanical assessment of the limpet tooth: Unraveling the secrets behind Nature's strongest material
16:30-17:45	Social/Poster discussions before tram arrives at 18:00	

Friday May 3rd, 2024

TIME	NAME	TITLE
8:00		Poster viewing
SESSION 5: Simulations and modelling of mechanical behavior *Chair: Petr Hauslid*		
8:30	Sandrine Brochard (Invited)	Structure, stability and mechanical properties of small metallic nanoparticles: insights from first-principles simulations
9:00	Mor Levi	Mechanical Properties of Nickel-Platinum Nanoparticles Fabricated by Solid-State Dewetting Synthesis
9:20	Miljan Dasic	Normal Dynamics - method development and applications
9:40	Frederik Van Loock	Amorphous plasticity at the mesoscale: development of a shear transformation zone-based numerical model
10:00	COFFEE BREAK	
SESSION 6: Managing mechanical data *Chair: Tamara Aleksandrov*		
10:30	Xufei Fang	Impact of room-temperature engineered dislocations on the mechanical properties in oxides
10:50	David Mercier	Dataflow Development and Machine Learning for Nanoindentation Data Analysis
11:10	Ulrich Kerzel	Transformation towards a digitized materials science laboratory
11:30	LUNCH and POSTER SESSION	
SESSION 7: Nanoscale deformation mechanisms and size effects *Chair: Daniel Kiener*		
13:00	Xie Zhuocheng (Invited)	Plasticity in topologically close-packed phases: Insights from nanomechanical testing and atomic-scale modelling
13:30	Maria Watroba	Micromechanical behavior of nanoporous electrodeposited Zn coating
13:50	Sina Zarepakzad	Investigating Mechanical Properties of Silicon Nanowires: Scale Effect Revisited
14:10	Selim Hanay	What can nanomechanical mass spectrometry tell us about nanoparticles?
14:30	Jonathan Zimmerman	Mass Particle Compression, or: How I learned to stop doing in-situ nanomechanical tests and love ex-situ ones

Normal Dynamics - method development and applications

Miljan Dašić*[1,2], Antonio Cammarata[1], and Paolo Nicolini[3]

[1]Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, 16627 Prague, Czech Republic – Czech Republic

[2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade – Pregrevica 118, 11080 Belgrade, Serbia, Serbia

[3]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 18200 Prague, Czech Republic – Czech Republic

Abstract

Normal Dynamics (*ND*) is a nanomechanical simulation method, the core of which is integration of the Newton's classical mechanics equations of motion, by adequately sampling the reciprocal space. Adequate sampling strategies and their capability of producing dynamical trajectories at the *ab initio* level with low computational demand will be discussed. *ND* method enables to: (1) obtain a systematic improvement of the accuracy, (2) to fine tune the computational resources' demand, and (3) to consider the atomic distortions happening across large distances, without the need of using large unit cells.
Theoretical background of the *ND* method is based on determining the phonon structure of a material. We will present several case studies which illustrate the method's applicability and computational performance. It will be explained that this simulation method has a general orientation, and it can be used for simulating: (a) periodic, (b) semiperiodic, and (c) finite systems (such as (a) crystals, (b) slabs, and (c) molecules).

Authors have implemented the *ND* method in the *Fortran* programming language (thus achieving high computational efficiency), and named the developed software - *PINDOL* (Phonon-Inspired Normal Dynamics of Lattices). *PINDOL* is an open-source software package for performing atom dynamics in the NVE and NVT ensembles (link for the free download: https://github.com/acammarat/pindol).

*Speaker

Exploring influence of water on the friction on two dimensional surfaces

Igor Stankovic*[1], Olivier Noel[2], and Miljan Dašić[1]

[1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun – Serbia

[2]Institut des Molécules et Matériaux du Mans – Le Mans Université, Institut de Chimie - CNRS Chimie, Centre National de la Recherche Scientifique – France

Abstract

This presentation explores water's influence on dynamic tribological contact in two systems: hydrophilic monolayer MoS2 and hydrophobic graphite interfaces. We reveal distinct stick-slip patterns at atomic resolution in the MoS2 system. Simulations highlight water's role in preventing prolonged slips by maintaining separation between solids. We explore the influence of water in both fully immersed conditions and air, emphasizing capillary water effects. Shifting the focus to hydrophobic interactions, our investigation challenges the conventional understanding of water expulsion in such contacts. We introduce a mechanism involving a droplet produced within the sliding nano-contact through the accumulation of water adsorbed on the substrate. The presentation concludes by demonstrating that a full slip regime of the droplet on the hydrophobic substrate explains the experimental tribological behavior. This research advances our understanding of dynamic friction on water molecule-contaminated surfaces, offering implications for industrial applications.

*Speaker

Berlin 2024 – scientific programme

BP: Fachverband Biologische Physik

BP 10: Computational Biophysics II

BP 10.9: Talk

Tuesday, March 19, 2024, 12:00–12:15, H 0112

selection status for this contribution: according to the sessions' setting

Enhancing protein-ligand binding affinity via optimal selection of water molecules — •Miljan Dašić, Jindřich Fanfrlík, and Jan Řezáč — Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, 166 10, Prague, Czech Republic

Accurate and fast determination of protein-ligand (P-L) binding affinity represents a foundational problem of computational biophysics. A promising solution is an universal physics-based scoring function **SQM2.20** based on semi-empirical quantum-mechanical computational methods. Its performance has been rigorously verified over a benchmark dataset **PL-REX** consisting of high-resolution crystal structures and trustworthy experimentally determined P-L affinities (10 diverse protein targets; 164 QM-optimized P-L complexes). Presence of water molecules has a significant impact on P-**L** binding affinity, via formation of hydrogen bond bridges. We have developed a computational tool which optimally selects waters enhancing the P-**L** binding affinity. Each of the ten protein targets comprises different crystals. Waters present in all of them represent the input for selection procedure. Such procedure includes clustering and comparison of waters contained in clusters with waters present in one selected reference crystal. Presence of optimally selected waters improves the correlation with experimental data. We investigated the sensitivity of scoring on the geometry of crystals. For each protein target, we determined the best reference crystal which maximizes the scoring results.

Keywords: protein-ligand binding affinity; semiempirical quantum-mechanical methods; physics-based scoring function; PL-REX benchmark dataset; impact of water molecules

Berlin 2024 – scientific programme

CPP: Fachverband Chemische Physik und Polymerphysik

CPP 21: Poster II

CPP 21.18: Poster

Tuesday, March 19, 2024, 18:00–20:00, Poster E

selection status for this contribution: according to the sessions' setting

Molecular dynamics study on the impact of water distribution on nanoscopic friction in case of monolayer MoS_2 — •Miljan Dašić[1, 2] and Igor Stankovic[2] — [1]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, 166 10, Prague, Czech Republic — [2]Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We have designed and applied a molecular dynamics (MD) simulation setup for the study of nanoscopic frictional phenomena in case of monolayer MoS_2. Our design represents a typical AFM experiment, comprising an amorphous SiO_2 probe in tribo-contact with a monolayer crystalline MoS_2 plate. Based on experimental conditions, we implemented two clearly distinguishable setups, regarding the water distribution: (1) large quantity of water - SiO_2 probe is fully immersed in water and surrounded by water molecules, and (2) ambient water - water coating is attached to the probe, which is surrounded by lateral vacuum gaps. We determined the force-distance characteristics of a fully-immersed probe at several temperatures, revealing that some water molecules get trapped in the probe-plate gap, with their number decreasing as temperature increases. We obtained well-defined stick-slip friction loops via sliding simulations. Considering the slip regime: fully-immersed probe mainly moves in single-slip regime, while ambient water distribution promotes multiple-slips. Amount of water, and especially its distribution, strongly influence the stick-slip frictional behaviour of the studied tribosystem.

Keywords: nanotribology; molecular dynamics; stick-slip friction; monolayer molybdenum disulfide; impact of water

Berlin 2024 – scientific programme

CPP: Fachverband Chemische Physik und Polymerphysik

CPP 15: Poster I

CPP 15.20: Poster

Monday, March 18, 2024, 18:00–20:00, Poster C

selection status for this contribution: according to the sessions' setting

The simulations of structural, thermodynamical, and mechanical characteristics of the mixture of ionic liquid and water using molecular dynamics: example of $[bmim]^+[PF_6]^-$ ionic liquid — •Mateja Jovanović[1,2], Miljan Dašić[1,3], and Igor Stanković[1] — [1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — [2]Institute of Technical Sciences of SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — [3]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo nam. 2, CZ-16610 Prague 6, Czech Republic

We present a study of the structural, thermodynamical, and mechanical properties of an ionic liquid 1-Butyl-3-methylimidazolium hexafluorophosphate $[bmim]^+[PF_6]^-$ water mixtures. Our simulation setup allows varying parameters of the system: temperature, concentration of ionic liquid, and shear rate of the system. We report significant changes compared to neat water or ionic liquids in the boiling temperature, diffusion coefficient, and viscosity. Even modest molar fractions of $[bmim]^+[PF_6]^-$ significantly affect the boiling point. The self-diffusion coefficient of water for the system with a lower concentration of ionic liquid is similar to the self-diffusion coefficient of neat water, and it decreases with increasing concentration of ionic liquid. Viscosity is investigated using equilibrium Green-Kubo relation and non-equilibrium molecular dynamics. In both cases, the viscosity coefficient increases with the increasing weight fraction of ionic liquid.

Keywords: ionic liquids; molecular dynamics; water; phase properties; transport

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CONTENTS

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View Abstract

CONTROL ID: 3831414
PRESENTATION TYPE: Early Career Researcher Poster
CURRENT TOPIC: Nanotribology

TITLE: Molecular Dynamics Investigation of the Nanoscopic Friction on Monolayer MoS_2 in the Presence of Water

AUTHORS (LAST NAME, FIRST NAME): Stankovic, Igor[1]; Dašić, Miljan[1]
INSTITUTIONS (ALL): 1. Scientific Computing Laboratory - Center for the Study of Complex Systems, Institute of Physics Belgrade, Zemun, Belgrade, Serbia.

ABSTRACT BODY:

Body: In the current work, molecular dynamics (MD) simulations are employed to study the nanoscopic friction on monolayer MoS2 in the presence of water. The simulation setup mimics atomic force microscope (AFM) experiments by using an amorphous probe made of SiO2, a monolayer MoS2 plate, and water molecules in between to simulate conditions due to air humidity. Two systems are compared, with a probe fully immersed in water and surrounded by water, and a water capillary around the probe. In the latter case, the stick-slip friction behaviour is pronounced and increases with the normal load. This study demonstrates that water content in the nanoscopic tribosystem of the MoS2 surface-SiO2 probe significantly impacts the probe's lateral and longitudinal movements, and therefore, its stick-slip behaviour.

KEYWORDS: Friction:Friction Mechanisms, Friction:Stick-Slip, Lubricants:Water, Water-Based.
Biography (limit 750 characters-about 100 words): Dr Igor Stanković obtained his PhD at the Technical University of Berlin in physics in 2004. He worked as Senior Simulation Engineer at Toyota Motor Europe in Brussels. Since 2009, he has been the Principal Research Fellow at the Institute of Physics in Belgrade. He is visiting professor at Technical University Federico Santa Maria Chile and a Fulbright visiting scholar at the University of California Merced. His research interests are application-driven and include computational nanotribology, ionic liquids (IL), and modelling AFM experiments. He has authored 35 journal papers, citations of more than 500, and h-index=13.
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P8

INFLUENCE OF WATER QUANTITY ON THE NANOSCOPIC FRICTION ON MONOLAYER MOS_2 INVESTIGATED WITH MOLECULAR DYNAMICS

Miljan Dašić[1], Igor Stanković[2]

[1] Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade (SRB)

* Corresponding author: mdasic@ipb.ac.rs

We have developed and utilized a molecular dynamics (MD) simulation setup in order to investigate the nanoscopic friction on monolayer crystalline MoS2, in the presence of two principally different quantities of water. Our simulation setup mimics a standard AFM experiment - comprising an amorphous SiO2 probe and a monolayer MoS2 sample. Presence of two different quantities of water in our simulations matches experimental conditions of: (1) air humidity (formation of a water *capillary* around the probe, without a full layer of water formed between the probe and the sample), and (2) *full water layer* (probe is fully immersed into water).

We conducted two modes of simulations: mode 1 - vertical approach (along the z- axis) of the SiO2 probe towards the MoS2 plate, and mode 2 - lateral sliding (along the x- axis) of the MoS2 plate. We have obtained trapped water molecules in the probe-sample gap in all mode 1 simulations, where their number drops with the temperature increase. Using mode 2 simulations, we obtained well-defined stick-slip friction curves. We found that an increase of the normal load applied on the probe leads to a better pronounced stick-slip behaviour, as seen in AFM experiments. Simulated probe-sample system with *capillary water* exhibits a lower friction coefficient than the system with *full water layer*, as a consequence of vacuum instead of water, surrounding the probe.

Our simulation setup includes quite a large number of atoms – 94163 in total, out of which there are 23497 water molecules (in case of *full water layer*). Taking into account the number of simulated atoms, it was necessary to make use of the NVIDIA-GPU acceleration. Our supercomputer *PARADOX* at the *Institute of Physics Belgrade* (SRB), on which we carried out simulations, has a significant number of nodes, with 16 GPU processors on each node and we were extensively employing them.

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C O N F I R M A T I O N

This is to confirm the participation of

Dr. Miljan Dasic

at the DPG Spring Meeting in Dresden (SKM23), March 26 - 31, 2023

with the talk:

"**Nanoscopic Friction on Monolayer *MoS_2* in Presence of Water Investigated with Molecular Dynamics**"

and the poster:

"**Tribological Properties of Selected Vanadium Oxides Investigated with *ReaxFF* molecular dynamics**"

The conference fee of 220,00 € has been paid.

Beatrice Hensel
Conference Management
Deutsche Physikalische Gesellschaft e. V.

Bad Honnef, March 31, 2023

Nanoscopic Friction on Monolayer MoS_2 in Presence of Water Investigated with Molecular Dynamics — •Miljan Dašić and Igor Stanković — Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We have implemented and applied a molecular dynamics (MD) simulation setup in order to study the nanoscopic friction on monolayer MoS_2 plate in the presence of different quantities of water. Our setup mimics a standard AFM experiment, including an amorphous SiO_2 probe, a monolayer crystalline MoS_2 plate, and water molecules in-between. Presence of water molecules matches experimental conditions of air humidity. We studied two different quantities of water: (1) *full water layer* - SiO_2 probe is fully immersed in water and surrounded by water molecules, and (2) *capillary water* - water forms a capillary around the SiO_2 probe, with lateral vacuum gaps. We conducted two modes of simulations: vertical approach of SiO_2 probe towards MoS_2 plate and lateral sliding of SiO_2 probe. There are always *trapped* water molecules in the gap between the probe and the plate; their number drops with the increase of temperature. We have obtained well-pronounced *stick-slip* friction loops; we found that an increase of the applied normal load leads to the more pronounced stick-slip behaviour, as seen in AFM experiments. The amount of water present in the studied nanoscopic tribosystem has a pronounced impact on the stick-slip frictional behaviour.

Part: CPP
Type: Talk
Topic: Polymer and Molecular Dynamics, Friction and Rheology
Email: mdasic@ipb.ac.rs
Submitted: Wed Nov 30 18:50:24 2022
Changed: Thu Dec 1 14:42:51 2022

Part: CPP

Number in Part: 286

Session:

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Contribution submission to the conference SKM 2023

Tribological Properties of Selected Vanadium Oxides Investigated with *ReaxFF* molecular dynamics — •Miljan Dašić[1,2], Ilia Ponomarev[1], Tomaš Polcar[1], and Paolo Nicolini[1] — [1]Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, Prague 6, 16627, Czech Republic — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Providing effective lubrication at high temperatures/pressures and in oxidative environments is relevant for various industrial applications, such as turbomachinery and cutting tools. Promising solutions are oxidation-resistant hard coatings consisting of binary or ternary films (e.g., $Cr-N$, $Ti-N$, $Cr-Al-N$, $Ti-Al-N$) doped with vanadium. The amount of oxygen present in an oxidative environment can be varied, leading to different vanadium oxide stoichiometries. We investigated tribological performance of under-oxidized vanadium lubricants, selected based on available experiments. We conducted a *ReaxFF* molecular dynamics study on selected stoichiometries {V_2O_3, V_3O_5, V_8O_{15}, V_9O_{17}, VO_2} at elevated temperatures {600, 800, 1000} [K] and pressures {1, 2, 3, 4} [GPa]. Our tribosystem consists of two rigid V_2O_5 layers, and a vanadium oxide in-between. At a fixed temperature, we did not notice significant changes of the friction coefficient with stoichiometry. All considered stoichiometries provide effective lubrication. Our study is relevant and interesting for the design of vanadium doped oxidation-resistant hard coatings.

Part: CPP
Type: Poster
Topic: Polymer and Molecular Dynamics, Friction and Rheology
Email: mdasic@ipb.ac.rs

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11th International Conference of The Balkan Physical Union

28 August – 1 September 2022, Belgrade, Serbia

THIS CERTIFIES THAT

MILJAN DAŠIĆ

he/she presented contribution **S04-AMP-100** with title

Tribological Properties of Selected Vanadium Oxide Stoichiometries Studied with Reactive Molecular Dynamics as **Oral presentation**.

Prof. Dr. Dragoljub D. Dimitrijević
Chair of the BPU11 LOC

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he/she presented contribution **S06-CMPSP-102** with title

Influence of the Size of Cation on the Structure and Tribological Properties of Ionic Liquids Studied with Molecular Dynamics as **Oral presentation**.

Prof. Dr. Dragoljub D. Dimitrijević
Chair of the BPU11 LOC

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Prof. Dr. Goran Djordjevic
President of the BPU

Contribution ID: **29** Contribution code: **S04-AMP-100** Type: **Oral presentation**

Tribological Properties of Selected Vanadium Oxide Stoichiometries Studied with Reactive Molecular Dynamics

Providing effective lubrication at high temperatures/pressures and in oxidative environments is relevant for various industrial applications, such as turbomachinery and cutting tools [1,2]. Promising solutions for such conditions are oxidation-resistant hard coatings consisting of binary or ternary films (Cr-N, Ti-N, Cr-Al-N, Ti-Al-N) doped with an additional element which can diffuse to the surface of the coating and form an oxide layer that serves as a lubricant. Vanadium became a popular dopant since its oxides melt at considerably low temperatures, hence providing liquid lubrication.

The amount of oxygen present in an oxidative environment can be taken as a study parameter, leading to the consideration of different vanadium oxide stoichiometries. This study aims to explore the tribological performance of under-oxidized vanadium lubricants, selected in accordance with available experimental studies [3].

We present a reactive molecular dynamics study on the tribological properties of five vanadium oxide stoichiometries {V_2O_3, V_3O_5, V_8O_{15}, V_9O_{17}, VO_2} at elevated temperatures {600, 800, 1000} [K] and pressures {1, 2, 3, 4} [GPa]. Our tribological system consists of two rigid V_2O_5 layers, modeling two solid surfaces in a tribocontact, and a vanadium oxide with stoichiometry labeled as V_xO_y, confined between them. Under the imposed working conditions, all studied vanadium oxides were amorphous.

We have employed an atomistic model within the *ReaxFF* (reactive force field) potential to describe the interactions of vanadium and oxygen atoms. Sliding simulations were implemented in the *reax/c* package of the *LAMMPS* code [4].

By applying a linear fit on the dependence of the sliding force F_x on the normal load F_z:

$$\mathrm{F}_x = COF \cdot F_z + F_x^0,$$

we extracted the coefficient of friction COF and the sliding force at zero load F_x^0 (adhesion component of the friction force). At a fixed temperature, we did not notice significant changes of the friction coefficient with stoichiometry. The values which we obtained for the COF (~0.2 at 600 K, ~0.15 at 800 K and ~0.1 at 1000 K) are in good agreement with the previously determined results for amorphous V_2O_5 lubricant at the same temperatures [5]. We concluded that all considered V_xO_y stoichiometries (i.e., under-oxidized vanadium) are going to be an effective lubricant. The friction coefficient COF decreases with the increase of the temperature. We observed the increasing trend of the adhesion-related offset of the friction force F_x^0 with the decrease of the oxygen content in V_xO_y lubricants and explained it by the more-pronounced tendency of vanadium atoms from V_xO_y to bond with oxygen atoms from V_2O_5 in oxygen-poorer environments.

Our study on vanadium oxide lubricants provides a reference which is relevant for the design of vanadium doped oxidation-resistant hard coatings.

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Presenter: Dr DAŠIĆ, Miljan (Scientific Computing Laboratory, Center for the Study of Complex Systems,Institute of Physics Belgrade, University of Belgrade)

Session Classification: S04 Atomic and Molecular Physics

Track Classification: Scientific Sections: S04 Atomic and Molecular Physics

Contribution ID: **42** Contribution code: **S06-CMPSP-102** Type: **Oral presentation**

Influence of the Size of Cation on the Structure and Tribological Properties of Ionic Liquids Studied with Molecular Dynamics

Ionic liquids (ILs) are two-component systems composed of large asymmetric and irregularly shaped organic cations and anions. Physical properties of ILs like negligible vapour pressure, high-temperature stability, high ionic conductivity and also a great variety of ILs and their mixtures highlight them as potentially relevant to lubrication [1, 2]. A large number of variations in IL composition is possible, estimated at the order of magnitude of 10^{18} different ILs. From their variety stems the possibility of tuning their physicochemical properties which can affect lubrication, such as viscosity, polarity, surface reactivity. Hence, it would be advantageous to figure out general relations between the molecular structure and tribological properties of ILs.

In this study, we investigate a generic tailed-model (TM) of ILs which includes: an asymmetric cation consisting of a positively charged head ($\sigma_C = 5$) and a neutral tail of variable size ($\sigma_T = 3, 5, 9$) and a large spherical negatively charged anion ($\sigma_A = 10$). It represents a more realistic model compared to the simplest one, the so called Salt Model (SM) [3, 4]. We figured that, although simple, TM model results in striking differences in equilibrium bulk structure of IL governed by the tail size relative to cationic head: (i) simple cubic lattice for the small tail, (ii) liquid-like state for symmetric cation-tail dimer, and (iii) molecular layer structure for the large tail. A mutual feature of all investigated model ILs is a formation of the fixed (stable) layer of cations along solid plates.

We have investigated the influence of the size of the cationic tail on the response of three ILs to confinement and mechanical strain, using molecular dynamics simulations in the *LAMMPS* code [5]. Tribological properties of three IL models are compared in and out of equilibrium. We have related the evolution of normal force with inter-plate distance to the changes in the number and structure of confined IL layers. A mutual feature of all investigated model ILs is a formation of the fixed (stable) layer of cations along the solid plates. The fixed layer formation is a result of strong Lennard-Jones interaction between the plates and ions. A consequence of the fixed layer stability is a steep rise of the normal force at small interplate gaps. The steep rise of the normal force is an effect useful for preventing solid-solid contact and accompanying wear.

Understanding the interplay between different processes in thin lubricant films is important due to the conflicting demands imposed on how IL lubricant should behave in dynamic confinement: high load-carrying capability requires strong adsorption to the surface, while low friction requires low viscosity.

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Primary authors: Dr STANKOVIĆ, Igor (Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade); DAŠIĆ, Miljan (Scientific Computing Laboratory, Center for the Study of Complex Systems,Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, 11080, Serbia)

Presenter: DAŠIĆ, Miljan (Scientific Computing Laboratory, Center for the Study of Complex Systems,Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, 11080, Serbia)

Session Classification: S06 Condensed Matter Physics and Statistical Physics

Track Classification: Scientific Sections: S06 Condensed Matter Physics and Statistical Physics

Contribution ID: **43** Contribution code: **S06-CMPSP-229** Type: **Poster presentation**

Tubular structures of magnetic particles: platform for curvilinear nanomagnetism

We review tubes [1,2] consisting of magnetic dipolar particles as a model for magnetic nanostructures and show, in particular, how to obtain anti-ferromagnetic states. The tubular assemblies of magnetic particles can be realized with different thickness, length, and lattice structures. The universality of dipolar interaction concerning the length scale allows the realization of these systems both at the macro scale as dipolar rotors and mesoscale using magnetic microspheres. Our system consists of tubes created by the assembly of dipolar spheres. The cylindrical topology results in the breakup of degeneracy observed in planar square and triangular packings. As far as the ground state is concerned, the tubes switch from circular to axial magnetization with increasing tube length. All magnetostatic properties found in magnetic nanotubes, in which the dipolar interaction is comparable to or dominant over the exchange interaction, are reproduced by the dipolar tubes including an intermediary helically magnetized state. Besides, we discuss the antiferromagnetic phase resulting from the square arrangement of the dipolar spheres and its interesting vortex state [2]. The proposed system should enable research of tubular magnetic nano-devices at scales that are more accessible for observation simultaneously avoiding material imperfections, existing in solid-state counterparts.

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Primary authors: Dr STANKOVIĆ, Igor (Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade); DAŠIĆ, Miljan (Scientific Computing Laboratory, Center for the Study of Complex Systems,Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, 11080, Serbia); Prof. GARCIA, Carlos (Departamento de Física & Centro Científico Tecnológico de Valparaíso-CCTVal, Universidad Técnica Federico Santa María)

Presenter: Dr STANKOVIĆ, Igor (Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade)

Session Classification: P06 Condensed Matter Physics and Statistical Physics

Track Classification: Scientific Sections: S06 Condensed Matter Physics and Statistical Physics

Contribution ID: **45** Contribution code: **S06-CMPSP-228** Type: **Poster presentation**

Non-equilibrium molecular dynamics investigation of a model ionic liquid lubricant for heavy-duty applications

In the current work, we present a modeling approach for simulating mesoscopic phenomena related to lubrication. Our geometry allows a variable confinement gap and a varying amount of lubricant in the gap. We have implemented and compared several coarse-grain molecular dynamics descriptions of an ionic liquid (spherical model and model with cation tail) as a lubricant that can expand into lateral reservoirs. The results have revealed two regimes of lubrication, and elastohydrodynamic one under low loads and one with low, velocity-independent specific friction, under high loads. The observed steep rise of normal forces at small plate-to-plate distances is an interesting behavior that could potentially be exploited for preventing solid-solid contact and wear.

Primary authors: STANKOVIĆ, Igor (Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade); DAŠIĆ, Miljan (Scientific Computing Laboratory, Center for the Study of Complex Systems,Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, 11080, Serbia)

Presenter: STANKOVIĆ, Igor (Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade)

Session Classification: P06 Condensed Matter Physics and Statistical Physics

Track Classification: Scientific Sections: S06 Condensed Matter Physics and Statistical Physics

ПРИЛОГ 6

Цитираност

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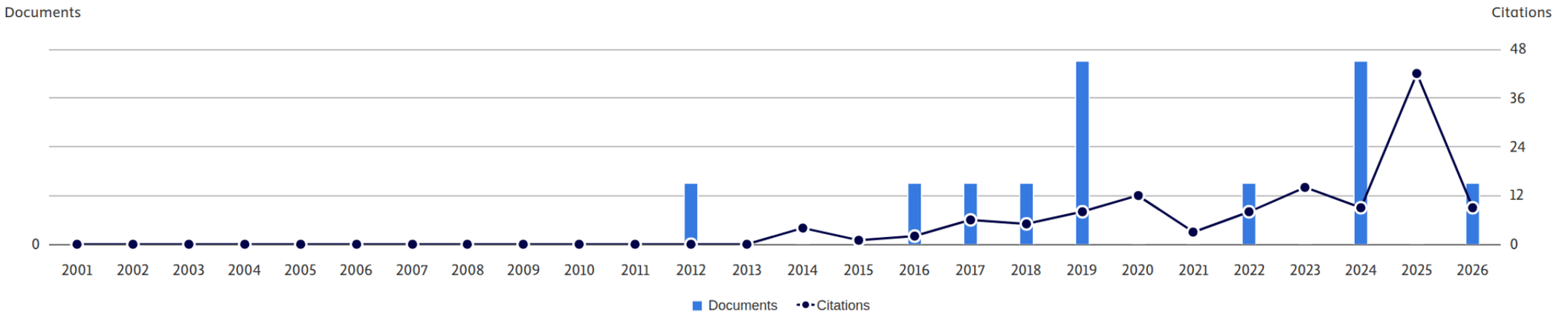

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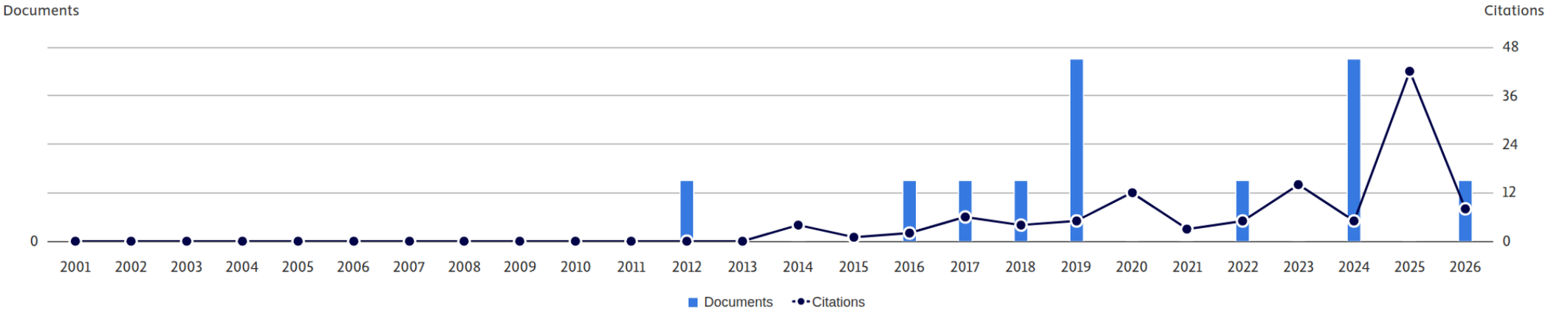

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2	Role of Trapped Molecules at Sliding Conta...	2024	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9
3	Effects of Water Content on the Transport ...	2024	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9
4	Tribological properties of vanadium oxides...	2022	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12
5	A platform for nanomagnetism-assembled...	2019	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9
6	Molecular dynamics investigation of the in...	2019	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20
7	Influence of confinement on flow and lubri...	2018	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6
8	Molecular dynamics investigation of a mo...	2017	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	22
9	Structure and cohesive energy of dipolar h...	2016	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	0	6
10	Minimum drop-loss design of microphoton...	2012	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	1	1	2	1	15

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Награде и признања

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Miljan Dašić Wins IPB's Student Prize

Monday, 20 July 2020

SCL's Miljan Dašić has won the IPB's Student Prize for the best doctoral thesis completed at IPB during 2019. The award was made for a high-quality research that enables understanding of Modeling the Behaviour of Confined Dipolar and Ionic Systems. The research was conducted under supervision of Dr. Igor Stanković and has resulted in five publications in international journals. The members of the Prize Committee were Dr. Marija Mitrović Dankulov, Dr. Branislav Cvetković and Dr. Nenad Vranješ.

We congratulate Miljan on this achievement.

News

30 May 2024
SCL Online Seminar by Jasper van Wezel

28 May 2024
IPB Seminar by Dejan Stojković

23 May 2024
SCL Online Seminar by Doron Cohen

16 May 2024
IPB Colloquium by Matej Krajnc

13 May 2024
SCL Seminar by Maxim Efremov

25 April 2024
SCL Online Seminar by Hareram Swain

18 April 2024
SCL Seminar by Veljko Janković

04 April 2024
SCL Seminar by Petar Mitrić

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TEDx Belgrade
x = independently organized TED event

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SCL's M. Dašić wins an avard from Chamber of Commerce and Idustry of Serbia

Thursday, 23 December 2021

SCL's researcher Miljan Dašić won an annual award for best PhD theses with applications in industry for the 2018/19 academic school year, awarded by the Chamber of Commerce and Industry of Serbia. The ceremony was held in the seat of the Chamber of Commerce and Industry of Serbia in Belgrade, on Thursday 23rd December 2021. M. Dašić's PhD thesis entitled

Modeling the Behaviour of Confined Dipolar and Ionic Systems (link)

was done at SCL under the mentorship of Dr Igor Stanković, in the research area of computational nanotribology. The main contributions include determining connections and consequences between structure and behaviour in classical systems of nanoparticles and molecules with long-range interactions.

This thesis was one of the 11 selected PhD theses for the award that recognizes novel solutions and significant contributions to industry, science, society and economy. However, due to the epidemic-related restrictions, this year the award was given for the best theses defended in the past two academic school years. A total number of 37 PhD theses, that came from 23 different faculties and 6 universities of the Republic of Serbia, was considered for the award.

News

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Subject COST Action CA21121 - Approval of application and Grant letter for ITC Conference grant E-COST-GRANT-CA21121-723b5467 - Dr Miljan Dašić

From COST Association Notification

To Miljan Dašić

Cc Marc Legros, Rose-Marie Tauzin-Melendo

Date 2024-06-04 19:02

cost
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Dear Dr Miljan Dašić,

Your application for a ITC Conference Grant with the following details:

- COST Action: CA21121
- Reference: E-COST-GRANT-CA21121-723b5467
- Grant requested: 1000.00 EUR
- Grant awarded: 1000.00 EUR
- Dates: 22/09/2024 - 27/09/2024

was approved by the MC of the COST Action.

Please find below the link for the Grant Letter that outlines your rights and duties and those of the Action Grant Holder.

https://e-services.cost.eu/activity/grants/723b5467-1e46-438e-879f-a5f7201df453/download/105903

A user guide providing an overview of the process is available here: https://www.cost.eu/grants_userguide. For further information about this procedure, please contact us or the Grant Awarding Coordinator Dr Marc Legros (marc.legros@cemes.fr).

Participant grants are non-commercial transactions, therefore, claims as such are not subject to V.A.T deduction. Taxes normally due or applicable with respect to the payment of the grant are not to be deducted from amounts payable to participants. It is the reponsibility of each participant to ensure that all amounts that they receive from COST funding are compliant with their national tax rules and obligations.

We thank you for your cooperation.

Kind regards,

Ms Rose-Marie Tauzin-Melendo

E-mail: ghm-cost@cemes.fr
Phone: 05 62 25 78 19

Best regards,

COST Association

ПРИВРЕДНА КОМОРА СРБИЈЕ
CHAMBER OF COMMERCE AND INDUSTRY OF SERBIA

додељује

ДИПЛОМУ

ДР МИЉАНУ ДАШИЋУ

ЗА ДОКТОРСКУ ДИСЕРТАЦИЈУ

МОДЕЛОВАЊЕ ПОНАШАЊА ПРОСТОРНО ОГРАНИЧЕНИХ
ДИПОЛНИХ И ЈОНСКИХ СИСТЕМА

одбрањену на Физичком факултету Универзитета у Београду
у школској 2018/19. години

Председник жирија

Проф. др Драган Ђуричин

Председник Привредне коморе Србије

Марко Чадеж

Београд, 23. децембар 2021. године

ПРИЛОГ 8

Сертификати

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

PRACE

CERTIFICATE OF ATTENDANCE

awarded to

MILJAN DAŠIĆ

for successful completion of the online PRACE Training Centre course

Introduction to MPI

May 25-27, 2021

on behalf of the organizing committee

Ing. Karina Pešatová, MBA

Head of Training and Education Department, IT4Innovations National Supercomputing Center

This event was partially supported by The Ministry of Education, Youth and Sports from the Large Infrastructures for Research, Experimental Development and Innovations project "e-Infrastruktura CZ – LM2018140" and partially by the PRACE-6IP project - the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823767. This work was also partially supported by the SGC grant No. SP2020/21 "Infrastructure research and development of HPC libraries and tools II", VŠB - Technical University of Ostrava, Czech Republic.

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

PRACE

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awarded to

Miljan Dašić

for successful completion of the online PRACE Training Centre course

Advanced MPI

October 19 - 21, 2021

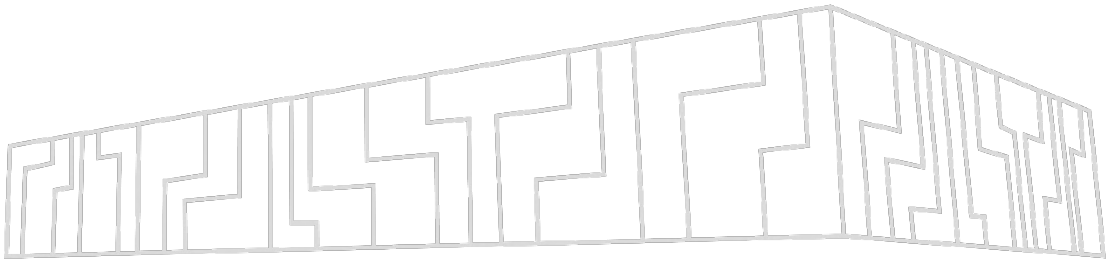
Karina Pešatová

Digitálně podepsal Karina Pešatová
Datum: 2021.10.22 11:52:44 +02'00'

on behalf of the organizing committee

Ing. Karina Pešatová, MBA

Head of Training and Education Department, IT4Innovations National Supercomputing Center



This event was partially supported by The Ministry of Education, Youth and Sports from the Large Infrastructures for Research, Experimental Development and Innovations project "e-Infrastruktura CZ – LM2018140" and partially by the PRACE-6IP project - the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823767. This work was also partially supported by the SGC grant No. SP2020/21 "Infrastructure research and development of HPC libraries and tools II", VŠB - Technical University of Ostrava, Czech Republic.

CERTIFICATE OF ATTENDANCE

This is to certify that

Miljan Dašic

attended the

15th European Biophysics CONGRESS

which was held in

Rome (Italy) from the 30th of June to the 4th of July 2025

The Organizing Secretariat

DOUBLE EM

UNIVERSITÄT PADERBORN

Paderborn Center for Parallel Computing

Universität Paderborn | PC2 | Warburger Str. 100, 33098 Paderborn, Germany

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Miljan Dašić

J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences

Confirmation of Participation

We hereby confirm that **Miljan Dašić** participated in

International Autumn School on CP2K-GROMACS for Multiscale Atomistic Simulation

at **Paderborn University** from **September 29** to **October 1**, **2025**. The 3-day event was jointly organized by the Paderborn Center for Parallel Computing (PC2) and the Center for Advanced Systems Understanding (CASUS). The program featured:

- Keynote lecture on GROMACS for force field based molecular dynamics by Prof. Dr. Helmut Grubmüller (Max Planck Institute for Multidisciplinary Sciences)
- Keynote lecture on CP2K for ab-initio molecular dynamics simulation by Prof. Dr. Thomas D. Kühne (Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, TU Dresden)
- Hands-on tutorials using CP2K and GROMACS for multiscale QM/MM atomistic simulation on HPC cluster systems at the Paderborn Center for Parallel Computing
- Poster session for scientific exchange focused on atomistic simulation.

The participant was engaged throughout the duration of the event.

Dr. Xin Wu

(on behalf of the Organization Committee)

ПРИЛОГ 9

Менторства

Univerzitet u Beogradu
Fizički fakultet

Simulacije strukturnih, termodinamičkih i mehaničkih karakteristika mešavine jonske tečnosti i vode metodom molekularne dinamike: primer $[bmim]^+[PF_6]^-$ jonske tečnosti

Mentori
Prof. dr Sunčica Elezović-Hadžić
Fizički fakultet

dr Miljan Dašić
Institut za fiziku u Beogradu

Student
Mateja Jovanović

septembar 2023

Zahvalnost

Ovaj rad je u potpunosti nastao u Laboratoriji za primenu računara u nauci, Instituta za fiziku u Beogradu, pod rukovodstvom dr Miljana Dašića. Želim da izrazim veliku zahvalnost Miljanu za uvod u kompleksan svet jonskih tečnosti i upotrebe opreme visokih računarskih performansi za naučna istraživanja. Takođe, želim da mu se zahvalim za sveobuhvatnu podršku tokom mog rada na master tezi, posebno zato što me je uputio u dobru naučnu praksu prezentovanja podataka i pisanja izveštaja.

Aleksandar Filipović i Matej Vučković

Ispitivanje tečno-čvrstog kontakta TM jonskih tečnosti i kristalne podloge metodom molekularne dinamike

U ovom radu ispitan je uticaj određenih faktora na tečno-čvrsti kontakt jonske tečnosi i podloge. Za jonsku tečnost korišćen je TM model (Tail Model – model sa repom) koji se sastoji od anjona i katjona povezanog sa neutralnim repom. Jednoslojna podloga ima kristalnu strukturu pravilne FCC (Face centered Cubic) 111 rešetke. Faktori koji su ispitani su asimetrija unutar jonske tečnosti, uticaj međusobne LJ (Lennard-Jones) interakcije između kristalne podloge i tečnosti, kao i uticaj početnog oblika kapljice jonske tečnosti. Posmatrana su dva početna oblika: sfera i kocka. Podloga je elektroneutralna, i Kulonova interakcija ne utiče direktno na tečno-čvrsti kontakt. Indirektni uticaj Kulonove interakcije manifestuje se kroz interakciju anjona i katjona unutar same tečnosti. Uticaj ovih faktora se izražava kroz promenu kohezije i adhezije. Ova promena se demonstrira promenom ugla kvašenja, pomoću kojeg su i izvedeni zaključci o uticaju ispitanih faktora.

Teorijski uvod

Jonske tečnosti su tečnosti organskih soli visoke asimetrije. Asimetrija potiče od velike razlike u veličini anjona i katjona, kao i od postojanja neutralnog repa povezanog sa katjonom. Posledice te asimetrije su niska temperatura topljenja i nemogućnost formiranja kristalne strukture (Dašić *et al.* 2019; Hayes *et al.* 2010). Tečnosti koje ćemo koristiti, po asimetriji liče na $[BMIM]^+[PF_6]^-$ i $[BMIM]^+[TFSI]^-$ jonske tečnosti. Kod $[BMIM]^+[PF_6]^-$ se očekuje potpuno, a kod $[BMIM]^+[TFSI]^-$ delimično kvašenje (Beattie *et al.* 2013; Bou-Malham i Bureau 2010; Wang i Priest 2013). Zbog mogućnosti varijacije velikog broja parametara u strukturi jonske tečnosti, postoji veliki broj različitih jonskih tečnosti. Procenjuje se da je taj broj reda veličine 10^{18} (Dold *et al.* 2013). Kvašenje ovih tečnosti potpuno varira u zavisnosti od vrste tečnosti i podloge koju ona kvasi. Parametri za koje ispitujemo uticaj na kvašenje su odnos veličina katjona, anjona i repova, jačina interakcije sa podlogom i početni oblik kapljice. Za simulacije interakcije nije bitna realna veličina atoma, već njihov Van der Valsov (VDW) radijus. To je prečnik sfere do čije površine najbliže može doći drugi atom.

Jedna vrsta interakcije do koje dolazi u simulacijama je Lenard-Džonsova interakcija (Lennard-Jones), u oznaci LJ interakcija (slika 1). Ona predstavlja pojednostavljen matematički model (1) međuatomskog potencijala. Ovako interaguju svi tipovi atoma u simulaciji. Ovaj potencijal zavisi od rastojanja između atoma i njihovih VDW radijusa. Sastoji se iz odbojnog i privlačnog dela (Dašić *et al.* 2019):

$$V = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad (1)$$

gde se prvi član odnosi na odbijanje, a drugi na privlačenje. Oznake su sledeće:

ϵ – dubina potencijala. Što je dublji potencijal to je jača interakcija (i odbojna i privlačna). U simulaciji postoje dva različita

Aleksandar Filipović (2002), Kragujevac, učenik 2. razreda Prve kragujevačke gimnazije

Matej Vučković (2002), Beograd, učenik 2. razreda Treće beogradske gimnazije

MENTOR: dr Miljan Dašić, Institut za Fiziku, Beograd

Mihajlo Srećković

Analiza magnetnih tubularnih struktura u homogenom magnetnom polju

U ovom radu ispitane su prstenaste i tubularne strukture sastavljene od nanočestica sa stalnim magnetnim dipolnim momentom u prisustvu eksternog vertikalnog (orijentisanog duž z-ose) homogenog magnetnog polja. Prstenaste strukture su strukture sastavljene od magnetnih nanočestica tako da se svi centri čestica nalaze na kružnici istog poluprečnika. Što se tiče tubularnih struktura, ispitane su AA i AB tube. AA tube su strukture sastavljene od magnetnih nanočestica koje se dobijajuređanjem prstenova jedan preko drugog duž z-ose, bez ikakve relativne rotacije između susednih prstenova. AB tube su strukture sastavljene od magnetnih nanočestica koje se dobijaju tako što se ređaju prstenovi jedan preko drugog sa relativnom rotacijom, tako da je svaka čestica koja čini jedan prsten pozicionirana između dve čestice iz prethodnog prstena. Razvijene su numeričke simulacije u programskom paketu MATLAB koje su zasnovane na metodu molekularne dinamike. Određeno je kritično eksterno magnetno polje pri kojem prstenasta struktura puca i razdvaja se u nanočestice od kojih je sastavljena. Ovo kritično polje raste sa povećanjem broja čestica do broja od 9 čestica, a zatim opada. Kod tubularnih struktura sastavljenih od 2 prstena se javljaju 2 kritična magnetna polja, ukoliko je broj čestica po prstenu veći od 4. Kada magnetna indukcija ima vrednost prvog kritičnog magnetnog polja, struktura puca i razdvaja se u prstenove od kojih je sastavljena, dok pri drugom kritičnom polju se razdvaja u individualne nanočestice.

Teorijski uvod

Čestice sa stalnim dipolnim momentom poznate su po svojim samoasemblirajućim osobinama. Magnetne strukture imaju široku primenu u nanotehnologiji (Whitesides i Grzybowski 2002), tako da je od izuzetnog značaja znati kako se one ponašaju. U biologiji, tubularne strukture su relevantni samoasemblirajući objekti koji su pronađeni u nekim vrstama bakterija i u ćelijskim mikrotubulama. Magnetne čestice se spontano mogu rasporediti tako da grade tubularne strukture (Stanković I., Dašić M. i Messina R. 2016.). U ovom radu posmatrana je dinamika magnetnih tubularnih struktura u spoljašnjem vertikalnom homogenom magnetnom polju. U tu svrhu razvijene su simulacije zasnovane na metodu molekularne dinamike u softverskom paketu MATLAB.

Magnetne čestice

Magnetne čestice se mogu definisati svojim dipolnim momentom i načinom na koji on interaguje sa magnetnim poljem. Čestica i sa dipolnim momentom $\boldsymbol{\mu}_i$ stavljena u magnetno polje indukcije $\boldsymbol{B}$ ima potencijalnu energiju

$$U_B^i = -\boldsymbol{\mu}_i \cdot \boldsymbol{B} \tag{1}$$

gde je U_B^i potencijalna energija interakcije sa magnetnim poljem. Iz jednačine (1) se može primetiti da će čestice težiti da poklope svoje dipolne momente sa magnetnim poljem kako bi minimizovale energiju. Ovo je jedna od bitnijih osobina magnetnih čestica.

Magnetne čestice takođe stvaraju oko sebe magnetno polje, čija se indukcija može odrediti jednačinom

Mihajlo Srećković (2005), Lebane, Nikole Pašića 2, učenik 3. razreda Gimnazije "Stojan Ljubić"
Mentori:
Dr Miljan Dašić, Institut za fiziku, Univerzitet u Beogradu
Nikola Petreski, Elektrotehnički fakultet, Univerzitet u Beogradu

ПРИЛОГ 10

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AS

Guest Editor of Special Issue

"Symmetry/Asymmetry in Condensed Matter Physics and Engineering Applications"

Dr. Miljan Dašić

1. Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia
2. Department of Computational Chemistry, J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, 18223 Prague, Czech Republic

MDPI

Basel, September 2025

S. Tochev

Stefan Tochev
Chief Executive Officer

Special Issue

Symmetry/Asymmetry in Condensed Matter Physics and Engineering Applications

Message from the Guest Editors

Recent rapid development of computational resources—both in terms of hardware and software—has made an enormous impact on the advances in the field of condensed matter physics as well as in various engineering applications. Especially, notable breakthroughs regarding Machine Learning (ML)—and, more broadly speaking, Artificial Intelligence (AI)—have enabled us to solve problems that we could not even imagine solving before. This has also led to the emergence of novel materials as well as new systems and phases, whose understanding requires novel approaches and new ideas. Symmetry/Asymmetry are fundamental concepts arising in nature, which manifest across physics and engineering. Research efforts considering those concepts are always modern and up-to-date, due to their universal relevance. By investigating symmetry/asymmetry, we can explore both established and emerging phenomena. This Special Issue of the journal *Symmetry* will focus on the interplay between the principles of symmetry/asymmetry and the fields of condensed matter physics and various engineering applications...

Guest Editors

Dr. Miljan Dašić

Dr. Sindy Julieth Rodriguez Sotelo

Prof. Dr. Sonja Grubišić

Deadline for manuscript submissions

31 May 2026

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About the Journal

Message from the Editor-in-Chief

Symmetry is ultimately the most important concept in natural sciences. It is not surprising then that very basic and fundamental research achievements are related to symmetry. For instance, the Nobel Prize in Physics 1979 (Glashow, Salam, Weinberg) was received for a unified symmetry description of electromagnetic and weak interactions, while the Nobel Prize in Physics 2008 (Nambu, Kobayashi, Maskawa) was received for the discovery of the mechanism of spontaneous breaking of symmetry, including CP symmetry. Our journal is named *Symmetry* and it manifests its fundamental role in nature.

Editor-in-Chief

Prof. Dr. Sergei Odintsov
1. ICREA, 08010 Barcelona, Spain
2. Institute of Space Sciences (IEEC-CSIC), C. Can Magrans s/n, 08193 Barcelona, Spain

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MDPI

ПРИЛОГ 11

Потврде о запослењу у иностранству

FACULTY OF ELECTRICAL ENGINEERING
Doc. Ing. Zdeněk Hurák, Ph.D.
DEPARTMENT OF CONTROL ENGINEERING

CTU
CZECH TECHNICAL UNIVERSITY IN PRAGUE

September 09, 2024, Prague

To whom it may concern:

Employment Certificate

We certify that Dr Miljan Dašić has worked at the Czech Technical University in Prague (CTU in Prague) as a postdoctoral researcher in the period 1.11.2019. - 31.12.2021.

During his employment at CTU in Prague, Dr Dašić participated in Czech-Austrian international project GF19-29679L (2019 - 2021) "Diffusion control reducing friction of nanocomposite materials", which was co-financed by the Czech Science Foundation (Grantová agentura České republiky – GAČR) and Austrian Science Fund (Fonds zur Förderung der wissenschaftlichen Forschung – FWF).

In case of any further information needed, feel free to contact us.

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Kamila Krupkova

Department of Control Engineering
Czech Technical University in Prague
Technicka 2, 16627 Praha 6, Czech Republic

ÚOCHB AV ČR
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PRACOVNÍ SMLOUVA

Ústav organické chemie a biochemie AV ČR, v. v. i.
Praha 6, Flemingovo nám. 2
zastoupen prof. RNDr. Janem Konvalinkou, CSc., ředitelem
(dále jen „zaměstnavatel")

a

MILJAN DAŠIĆ, Ph.D.
nar. 03.11.1990
bytem: Majora Marka 13, 352 50 Paraćin, Srbsko
číslo pasu / ID: 013941712
(dále jen „zaměstnanec")

uzavírají tuto

pracovní smlouvu:

I.

1. Pracovní poměr se sjednává na dobu určitou, do 28.02.2024
2. Zaměstnanec nastoupí do práce dnem 01.03.2023
3. Druh práce: postdoktorand
4. Místo výkonu práce: Praha
5. Zkušební doba se sjednává do 31.05.2023
6. Délku týdenní pracovní doby a rozvržení pracovní doby stanoví § 79 a násl. zákoníku práce, pracovní řád a kolektivní smlouva.
   Další ujednání o pracovní době: po vzájemné dohodě činí pracovní úvazek 100 %, tj. 8 hodin denně. Při tomto úvazku budete plně kmenovým zaměstnancem ústavu.
7. Zaměstnavatel bude přidělovat zaměstnanci práci podle pracovní smlouvy.
8. Zaměstnavatel vytvoří zaměstnanci podmínky pro úspěšné plnění pracovních úkolů, zejména zajistí bezpečnost a ochranu zdraví při práci.

občanského průkazu, zvýšení kvalifikace, jakož i okolnosti, které mohou mít vliv na výkon práce a plnění vzájemných povinností.

III.

1. Činnost výzkumných pracovníků, zejména jejich publikační aktivita a výsledky vědecké práce, bude pravidelně hodnocena Atestační komisí ÚOCHB AV ČR, v. v. i., jmenovanou ředitelem, přičemž závěr atestací, spočívající v nesplňování požadavků pro řádný výkon práce, může být důvodem k rozvázání pracovního poměru ze strany zaměstnavatele.

IV.

1. Zaměstnanec bere na vědomí, že u zaměstnavatele působí odborová organizace, se kterou byla uzavřena kolektivní smlouva.

2. Vzájemná práva a povinnosti, plynoucí z pracovního poměru, upravuje především zákoník práce, zákon o veřejných výzkumných institucích, zákon o Akademii věd ČR, Stanovy Akademie věd ČR, příslušná ustanovení občanského zákoníku; dále pak vnitřní předpisy zaměstnavatele, s nimiž byl zaměstnanec při nástupu do práce seznámen, a to kolektivní smlouva, organizační řád, pracovní řád, předpisy k zajištění bezpečnosti a ochrany zdraví při práci a požární ochrany, vnitřní mzdový předpis a další vnitřní předpisy upravující pracovněprávní vztahy.

3. Pracovní smlouva se vyhotovuje ve dvou výtiscích, z nichž jeden obdrží zaměstnanec a jeden zaměstnavatel.

4. Smluvní strany podpisem stvrzují souhlas s obsahem této pracovní smlouvy, zaměstnanec současně i převzetí jednoho jejího výtisku.

5. Tato smlouva stanovuje podrobnosti pracovního poměru mezi zaměstnancem a zaměstnavatelem, jehož základní rámec upravuje pracovní řád zaměstnavatele. Je – li ustanovení této smlouvy a ustanovení pracovního řádu v rozporu, použije se vždy přednostně ustanovení této smlouvy.

V Praze dne 01.03.2023

ÚSTAV ORGANICKÉ CHEMIE A BIOCHEMIE
AKADEMIE VĚD ČESKÉ REPUBLIKY, v.v.i.
Personální oddělení
Flemingovo nám. 2, 166 10 Praha 6
DIČ: CZ61388963
-2-

.....
zaměstnanec

.....
zaměstnavatel

ÚOCHB AV
IOCB PRAGUE

Ústav organické chemie a biochemie AV ČR, v.v.i.
Flemingovo nám. 2
166 10 Praha 6

DOHODA O ZMĚNĚ PRACOVNÍ SMLOUVY

ze dne 01.03.2023

MILJAN DAŠIĆ Ph.D.

nar. 03.11.1990

Na základě oboustranné dohody p r o d l u ž u j e m e Váš pracovní poměr **do 31.12.2024**, a to v souladu s „Dohodou o sjednávání pracovních poměrů na dobu určitou" uzavřenou mezi ÚOCHB AV ČR, v.v.i. a odborovou organizací dne 6.8.2013.

Ostatní náležitosti výše uvedené pracovní smlouvy ve znění pozdějších změn zůstávají v platnosti.

Tento doklad je nedílnou součástí pracovní smlouvy ze dne 01.03.2023

Smluvní strany podpisem stvrzují souhlas s obsahem této dohody, zaměstnanec současně i převzetí jednoho jejího výtisku.

V Praze dne 10.11.2023

ÚSTAV ORGANICKÉ CHEMIE A BIOCHEMIE
AKADEMIE VĚD ČESKÉ REPUBLIKY, v.v.i.
Personální oddělení
Flemingovo nám. 2, 166 10 Praha 6
DIČ: CZ61388963

-2-

.....
Zaměstnanec

.....
Zaměstnavatel

ÚOCHB AV ČR
IOCB PRAGUE

POPIS PRÁCE / JOB DESCRIPTION

Název pozice / Position: Postdoktorand

Oddělení / Department: Nekovalentní interakce

Vedoucí / Manager (Group Leader): Pavel Hobza

Třída / Salary category: V3

Jméno zaměstnance / Employee name: Miljan Dašić

Popis práce / Description:

Vývoj softwarového frameworku pro integraci semiempirických kvantově-mechanických výpočtů a korekcí pro nekovalentní interakce do komplexních výpočetních protokolů.

Speciální odpovědnosti / Special Responsibilities:
(dohoda o odpovědnosti, řízení motorového vozidla, etc.)

Funkce (jmenování) / Nominations:

Požadované kvalifikace / required qualifications:

Vzdělání Vzdělání / Education:	Ph.D.
Jazyky / Languages:	angličtina
Jiné / Other:	

Dne / Date: .....

Podpis zaměstnance / Signature (Employee): .....

Dne / Date: 23.2.2023

Podpis vedoucího / Signature (Manager, Group leader): .....

PRACOVNÍ SMLOUVA

uzavřená dle ust. § 33 a násl. zákona č. 262/2006 Sb., zákoník práce, ve znění pozdějších předpisů
(dále jen „Zákoník práce")

Zaměstnavatel:

Název:	Ústav fyzikální chemie J. Heyrovského AV ČR, v. v. i.
Sídlo:	Dolejškova 2155/3, 182 23 Praha 8
IČ:	613 88 955
Zastoupená:	prof. Martin Hof, Dr. rer. nat., DSc., Director

na straně jedné (dále jen „zaměstnavatel")

a

Zaměstnanec:

Os. číslo:	2199
Titul před jménem:	
Příjmení a jméno:	Dašić Miljan
Titul za jménem:	Ph.D.
Datum narození:	03.11.1990
Bydliště:	Majora Marka 13, 352 50 Paraćin

Státní příslušnost: **Srbsko**

na straně druhé (dále jen "zaměstnanec")

uzavírají tuto

PRACOVNÍ SMLOUVU

I.

1. **Druh práce:** **Vědecký asistent** **R0**

   Místo výkonu práce: **Praha**

   Pravidelné pracoviště pro účely cestovních náhrad: **Praha**

2. Dnem nástupu do práce je: **13.01.2025**

3. Pracovní poměr se sjednává **na dobu určitou do 31.12.2026**

4. Pracovní úvazek: **1** bude hrazen: **1.00**
   Prémie Lumina Quaeruntur **Timr** **574023**

5. Délka týdenní pracovní doby: **40**

   Úvazek může být v případě potřeby upravován podle vývoje Projektu a podmínek jeho poskytovatele.

6. Zkušební doba: **12.04.2025**
   a) se sjednává v délce trvání třech (3) měsíců ode dne vzniku pracovního poměru.

b) Zaměstnavatel i zaměstnanec mohou zrušit pracovní poměr ve zkušební době z jakéhokoliv důvodu nebo bez uvedení důvodu, a to písemným oznámení doručeným druhé smluvní straně.

7. **Mzdové zařazení:**
Zaměstnavatel se zavazuje vyplácet zaměstnanci za vykonanou práci mzdu ve výši stanovené zaměstnavatelem v souladu s ust. § 113 odst. 1 Zákoníku práce v mzdovém výměru.

8. **Dovolená:**
Zaměstnanci náleží dovolená na zotavenou podle zákoníku práce. Její celková délka činí pět týdnů ročně. Podrobnosti upravují ustanovení § 212 a násl. Zákoníku práce.

II.

1. Zaměstnavatel je povinen vytvářet zaměstnanci podmínky pro řádné plnění jeho pracovních úkolů a dodržovat ostatní podmínky stanovené právními předpisy, touto pracovní smlouvou a platnou kolektivní smlouvou.

2. Zaměstnanec přebírá odpovědnost za jemu svěřené věci v rámci výkonu práce (finanční zálohy, notebook, mobilní telefon, klíč), přičemž v případě ztráty nebo zničení věci je zaměstnanec povinen nahradit zaměstnavateli škodu způsobenou ztrátou či zničením svěřených věcí dle ust. § 255 Zákoníku práce. O předání svěřených věcí dle ust. § 255 Zákoníku práce bude mezi zaměstnancem a zaměstnavatelem uzavřen předávací protokol.

3. Zaměstnanec je povinen podle pokynů zaměstnavatele konat osobně, svědomitě, řádně a ve stanovené době jemu přidělenou práci, jež odpovídá druhu práce sjednanému v čl. I odst. 1 této pracovní smlouvy, náplni práce na příslušném projektu, řídit se přitom pokyny svého vedoucího, vnitřními předpisy zaměstnavatele, platnou kolektivní smlouvou, předpisy o bezpečnosti a ochraně zdraví při práci a dalšími předpisy vztahujícími se k práci jím vykonávané. S příslušnými předpisy byl zaměstnanec seznámen.

4. Zaměstnanec nesmí bez předchozího písemného souhlasu zaměstnavatele vykonávat výdělečnou činnost, která je shodná s předmětem činnosti zaměstnavatele. Zaměstnanec se zavazuje, že sjedná-li pracovní poměr k jinému zaměstnavateli k výkonu činnosti, která není shodná s předmětem činnosti jeho zaměstnavatele, oznámí tuto skutečnost zaměstnavateli bez zbytečného odkladu.

5. Zaměstnanec nesmí využívat výsledků dosažených v rámci této pracovní smlouvy pro jinou výdělečnou činnost.

6. Zaměstnanec se zavazuje zachovávat mlčenlivost o všech skutečnostech, o nichž se dozvěděl v souvislosti s plněním pracovních úkolů dle této pracovní smlouvy, a které jsou předmětem obchodního tajemství ve smyslu ust. § 504 zákona č. 89/2012 Sb., občanský zákoník, ve znění pozdějších předpisů. Zaměstnanec se zavazuje zachovávat mlčenlivost o všech skutečnostech týkajících se klientů zaměstnavatele, výsledků výzkumu, o nichž se dozvěděl v souvislosti s plněním pracovních úkolů podle této pracovní smlouvy.

7. Zaměstnanec souhlasí s vysíláním na pracovní cesty v tuzemsku i do zahraničí. Zaměstnanec je povinen hlásit zaměstnavateli veškeré změny v osobních údajích, k nimž dojde v průběhu trvání pracovního poměru, zejména změny v počtu vyživovaných osob, rozhodné údaje pro daňové přiznání a pro zdravotní a sociální pojištění, jakož i veškeré okolnosti, které mohou mít vliv na výkon práce a na nároky a povinnosti z pracovního poměru vyplývající.

8. Bude-li zaměstnanec vykonávat práci v jiném členském státě EU, je povinen požádat nejpozději 1 měsíc před odjezdem do zahraničí o vystavení „*Potvrzení o právních předpisech sociálního zabezpečení, které se vztahují na držitele*“ (tzv. formulář A1), jímž bude určeno, jaké právní předpisy sociálního zabezpečení se na zaměstnance budou vztahovat, pokud bude vykonávat práci mimo Českou republiku.

III.

1. Ostatní práva a povinnosti smluvních stran, vyplývající z této pracovní smlouvy, se řídí příslušnými ustanoveními zákoníku práce a dalšími předpisy upravujícími pracovně právní vztahy.

2. Sjednaný obsah této pracovní smlouvy lze měnit, dohodnou-li se zaměstnavatel a zaměstnanec na jeho změně. Změna musí být provedena písemně formou dodatku ke smlouvě.

3. Zaměstnanec prohlašuje, že byl seznámen s Informacemi o základních právech a povinnostech vyplývajících z pracovního poměru, s pracovními a mzdovými podmínkami, které obdržel v písemné formě. Při nástupu do práce byl zaměstnanec seznámen s pracovními povinnostmi, s interními předpisy zaměstnavatele a s předpisy k zajištění bezpečnosti a ochrany zdraví při práci a s protipožárními předpisy, jež musí při své práci dodržovat.

4. Pokud některé z ustanovení této smlouvy je nebo se stane neplatným či neúčinným, nebude to mít za následek neplatnost či neúčinnost této smlouvy jako celku ani jiných jejích ustanovení, pokud je takovéto neplatné či neúčinné ustanovení oddělitelné od zbytku smlouvy. Smluvní strany se zavazují neplatné či neúčinné ustanovení nahradit novým platným či účinným ustanovením, které svým obsahem bude co nejvěrněji odpovídat podstatě a smyslu původního ustanovení smlouvy.

5. Zaměstnanec byl řádně poučen o zpracovávání jeho osobních údajů, a to na základě plnění smlouvy, plnění právní povinnosti a/nebo jeho výslovného souhlasu. Podrobnosti stanoví Informace o zpracovávání osobních údajů, které zaměstnanec před podpisem této smlouvy obdržel.

6. Tato pracovní smlouva je připravena ve dvou vyhotoveních, zaměstnanec i zaměstnavatel obdrží po jednom vyhotovení.

V Praze dne 13.01.2025

Zaměstnanec
Dašić Miljan Ph.D.

V Praze dne 13.01.2025

ÚSTAV FYZIKÁLNÍ CHEMIE
J. Heyrovského AV ČR, v. v. i.
Dolejškova 2155/3, 182 23 Praha 8
IČO: 61388955 DIČ: CZ61388955

Zaměstnavatel:
prof. Martin Hof, Dr. rer. nat., DSc., ředitel

PRACOVNÍ NÁPLŇ

Zaměstnanec:

Os. číslo: 2199

Titul před jménem:

Příjmení a jméno: Dašić Miljan

Titul za jménem: Ph.D.

CZ - ISCO - kód: 21134 **Název:** Fyzikální chemici, chemici analytici

Oddělení: 19100006 **Název oddělení:** Odd. výpočetní chemie

POPIS JEDNOTLIVÝCH PRACÍ

Prémie Lumina Quaeruntur – 57 40 23

Výpočetní modelování enzymů a jejich dynamických shluků, implementace víceškálového rámce pro propojení molekulárních simulací enzymů a ligandů v dynamických enzymových shlucích s kinetickými modely metabolických drah, publikace výsledků a prezentace výstupů na mezinárodních konferencích.

Job description:

Computational modeling of enzymes and their dynamic assemblies, implementation of a multi-scale framework to couple molecular simulations of enzymes and ligands in dynamic enzyme assemblies with kinetic models of metabolic pathways, publication of results, and presentation of the work at international conferences.

Zaměstnanec vykonává podle operativního rozhodování nadřízeného případně i jiné úkony spadající do rámce dané odbornosti.

V Praze dne 13.1.2025

Zaměstnanec:

.....

Miljan Dašić

Zaměstnavatel:

ÚSTAV FYZIKÁLNÍ CHEMIE
J. Heyrovského AV ČR, v. v. i.
Dolejškova 2155/3, 182 23 Praha 8
IČO: 61388955, DIČ: CZ61388955

.....

prof. Martin Hof, Dr. rer. nat., DSc.
ředitel

Obdrží: zaměstnanec
personální oddělení