NAUČNOM VEĆU INSTITUTA ZA FIZIKU

Predmet: Molba za pokretanje postupka za reizbor u zvanje
viši naučni saradnik

Molim Naučni savet Instituta za fiziku da, u skladu sa Pravilnikom o postupku i načinu vrednovanja i kvantitativnom iskazivanju naučnoistraživačkih rezultata istraživača, pokrene postupak za moj reizbor u zvanje viši naučni saradnik.

Beograd, 11.04.2014. Mirjana Grujić-Brojčin

MIŠLJENJE RUKOVODIOCA PROJEKTA SA PREDLOGOM ČLANOVA KOMISIJE ZA PISANJE IZVEŠTAJA

Dr Mirjana Grujić-Brojčin zaposlena je u Centru za fiziku čvrstog stanja i nove materijale Instituta za fiziku u Beogradu, na projektima Ministarstva prosvete, nauke i tehnološkog razvoja:

- III45018 “Nanostrukturni multifunkcionalni materijali i nanokompoziti”,
- ON171032 “Fizika nanostrukturnih oksidnih materijala i jako korelisanih sistema”.

Pošto ispunjava sve uslove predviđene Pravilnikom za izbore naučno-istraživačka zvanja, saglasan sam sa pokretanjem postupka za reizbor dr Mirjane Grujić-Brojčin u zvanje viši naučni saradnik.

Predlog članova Komisije za pisanje izveštaja:

1. dr Maja Šćepanović, naučni savetnik, Institut za fiziku
2. dr Aleksandar Golubović, naučni savetnik, Institut za fiziku
2. Prof. dr Dejan Raković, redovni profesor, Elektrotehnički fakultet Univerziteta u Beogradu

Rukovodilac projekta

prof dr Zoran V. Popović

dr Mirjana Grujić-Brojčin
Biografija

Dr Mirjana Grujić-Brojčin, rođena je 1970. godine u Kragujevcu.

Diplomirala 1996. godine na Odseku za fizičku elektroniku, Smer za elektrotehničke materijale i tehnologije Elektrotehničkog fakulteta u Beogradu.

Odbranila je magistarsku tezu "Proračun molekularnih vibracija klastera jednoslojnih nanotuba" na temu na Elektrotehničkom fakultetu u Beogradu, smer Elektrotehnički materijali i tehnologije.

Doktorski rad pod naslovom "Optička spektroskopija oksidnih nanoprahova" odbranila je na Elektrotehničkom fakultetu u Beogradu 16. oktobra 2008. godine.

Od 16. decembra 1996. godine zaposlena je u Institutu za fiziku, Centar za fiziku čvrstog stanja i nove materijale.

U zvanje istraživač saradnik 24. aprila 2001. godine.

U zvanje viši naučni saradnik izabrana 14. oktobra 2009. godine.

Dr Mirjana Grujić-Brojčin angažovana je na sledećim projektima Ministarstva za prosvetu, nauku i tehnološki razvoj Republike Srbije:

- 1996-2000. god. projekat: “Fizika materijala” (rukovodilac prof. dr Zoran V. Popović)
- 2001-2005. god. projekat: “Fizika niskodimenzionih i nanometarskih struktura i materijala” (rukovodilac prof. dr Zoran V. Popović).
- 2006-2010. god. projekat MNTR Srbije br. 141047B “Fizika niskodimenzionih i nanometarskih struktura i materijala” (rukovodilac prof. dr Zoran V. Popović).
- 2008-2009. godine inovacioni projekat „Proizvodnja nanoprahova čistog i dopiranog anatasa vrhunskog kvaliteta pomoću sol-gel tehnologije“ (rukovodilac dr Aleksandar Golubović)
- od 2010. godine angažovana na projektima ON17032 "Fizika nanostrukturnih oksidnih materijala i jako korelisanih sistema" i III45018 "Nanostrukturni multifunkcionalni materijali i nanokompoziti" Ministarstva prosvete, nauke i tehnološkog razvoja.
- 2012-2013 godine inovacioni projekat "Proizvodnja visokokvalitetnih TiO_2 nanoprahova efikasnih u fotokatalitičkoj razgradnji organskih zagađivača" (rukovodilac dipl. inž. Dejan Ćukalović)
-

Takođe je bila angažovana na sledećim međunarodnim projektima:

- od 2004. godine bilateralni projekat "Raman Scattering and Photoluminescence from Semiconductor Nanoparticles", sklopljen između Instituta za fiziku čvrstog stanja Bugarske akademije nauka i Centra za fiziku čvrstog stanja i nove materijale IF,

- 2006-2009. godine – evropski projekat Centre of Excellence for Optical Spectroscopy Applications (OPSA-026283) in Physics, Material Science and Environmental Protection**,** u okviru FP6 programa (2006-2009),
- 2007-2008 na evropskom projekat *Controlling Mesoscopic Phase Separation – CoMePhS* , STREP FP6, No. 517039
- 2009-2012. godine na projektu bilateralne saradnje SCOPES sa Institutom za fiziku polimera Federalnim tehničkim institutom Cirih (ETH Zurich) Švajcarska
- od 2013. godine bilateralni projekat " Scientific and technological cooperation between Sapienza University of Rome and University of Belgrade in the area of Cultural Heritage ", sklopljenom između Instituta za fiziku Univerziteta u Beogadu i Univerziteta Sapienca u Rimu, Italija.

Dr Mirjana Grujić-Brojčin bavi se Ramanovom, fotoluminescentnom i infracrvenom spektroskopijom, kao i spektroskopskom elipsometrijom oksidnih nanoprahova i tankih filmova. Bavi se razvojem i usavršavanjem numeričkih modela vezanih za vibracionu spektroskopiju nanostrukturnih materijala, odnosno numeričko modelovanje vibracionih spektara, kao i numeričkim modelovanjem poroznosti nanoprahova. Od prošle godine, aktivno se bavi primenom metoda optičke spektroskopije u oblasti proučavanja i očuvanja kulturnih dobara.

Koautor je monografije "Optička svojstva nanomaterijala" (Z. D. Dohčević-Mitrović, M.J. Šćepanović, M. Grujić-Brojčin, Z. V. Popović), objavljene u izdanju Instituta za fiziku i Akademske misli, 2011. godine

Do sada je objavila preko 60 naučnih radova, od čega 35 u međunarodnim časopisima, 3 u nacionalnim, a 6 radova je izlagano po pozivu na međunarodnim i nacionalnim konferencijama.

Ovi radovi do sada su citirani preko 290 puta u međunarodnim časopisima (240 puta ne računajući autocitate), sa h-indeksom 8.

Dr Mirjana Grujić-Brojčin

Bibliografija 2009-2014.

I RAD U VRHUNSKOM MEĐUNARODNOM ČASOPISU – M21

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"Raman study of structural disorder in ZnO nanopowders"
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II RAD U VODEĆEM MEĐUNARODNOM ČASOPISU – M22

M. J. Šćepanović, M. Grujić-Brojčin, Z. D. Dohčević-Mitrović, Z. V. Popović
"Characterization of Anatase TiO2 Nanopowder by Variable-Temperature Raman Spectroscopy"
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III RAD U MEĐUNARODNOM ČASOPISU – M23

1
Z.V. Popović, Z. Dohčević-Mitrović, M. Šćepanović, M. Grujić-Brojčin and S. Aškrabić
"Raman scattering on nanomaterials and nanostructures"
Annalen Der Physik 523(1-2) (2011) 62-74
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2
M. Šćepanović, S. Aškrabić, M. Grujić-Brojčin, A. Golubović, Z. Dohčević-Mitrović, B. Matović and Z.V. Popović
Raman study of vanadium-doped titania nanopowders synthesized by sol-gel method
International Journal Of Modern Physics B 24(6-7) (2010) 667-675
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3
M. Šcepanović, M. Grujić-Brojčin, M. Mirić, Z. Dohčević-Mitrović and Z.V. Popović
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M23 (3)

4
M. Šcepanović, M. Grujić-Brojčin, D. Nesheva, Z. Levi, I. Bineva and Z.V. Popović
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IV RAD U VODEĆEM ČASOPISU NACIONALNOG ZNAČAJA - M51

1
Nenad Ž. Lazarević, Zorana D. Dohčević-Mitrović, Mirjana U. Grujić-Brojčin, Maja J. Šćepanović, Marko B. Radović, Zoran V. Popović
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M51 (2)

V MONOGRAFIJA OD NACIONALNOG ZNAČAJA - M41

1
Z. D. Dohčević-Mitrović, M.J. Šćepanović, M. Grujić-Brojčin, Z. V. Popović

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VI RAD U MEĐUNARODNOM ČASOPISU BEZ IMPAKT FAKTORA

1
Maja Šćepanović, Mirjana Grujić-Brojčin, Zorana Dohčević-Mitrović, and Zoran V. Popović
Investigation of vibrational and electronic properties of oxide nanopowders by spectroscopic methods
Journal of Physics: Conference Series **253** (2010) 012015

Ukupno: 6 x M21
1 x M22
6 x M23
1 x M51
1xM41
80

Диференцијални услов- Од првог избора у претходно звање до избора у звање виши научни сарадник	потребно је да кандидат има најмање XX поена, који треба да припадају следећим категоријама:		
		Неопходно XX=	Остварено
Виши научни сарадник	Укупно	48	80
	M10+M20+M31+M32+M33 M41+M42+M51 ≥	40	80
	M11+M12+M21+M22 M23+M24+M31+M32+M41+M42 ≥	28	73

За избор у научног саветника је потребно да је публикован један рад категорија M41-45 M51-52 на српском језику или језицима националних мањина

Dr Mirjana Grujić-Brojčin, CITIRANOST

Sum of the Times Cited: 291
Sum of Times Cited without self-citations : 242

H-factor 8

EXPORT DATE:18 Mar 2014 (Source: Scopus/Web of Science)

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Dohcevic-Mitrovic, Z.D., Šćepanović, M.J., Grujić-Brojčin, M.U., Popović, Z.V., Bošković, S.B., Matović, B.M., Zinkevich, M.V., Aldinger, F.
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PREGLED NAUČNO ISTRAŽIVAČKIH AKTIVNOSTI

Naučno istraživačka aktivnost dr Mirjane Grujić-Brojčin vezana je za istraživanja u oblasti fizike čvrstog stanja od 2009. godine odvijala se u nekoliko pravaca:

1. *Karakterizacija nanostrukturnih materijala, posebno modelovanje optičkih spektara oksidnih nanoprahova*
2. *Modelovanje optičkih i poroznih svojstava nanostrukturnih oksida za fotokatalitičke primene*
3. *Primena metoda optičke spektroskopije u izučavanju i zaštiti kulturnih dobara*

Dr Mirjana Grujić-Brojčin je autor i koautor preko 60 referenci, od čega je 35 radova publikovano u međunarodnim časopisima. Ovi radovi citirani su do sada preko 290 puta, odnosno 240 ne računajući autocitate.

1. Karakterizacija nanostrukturnih materijala, posebno modelovanje optičkih spektara oksidnih nanoprahova

Od 2004. godine dr Mirjana Grujić-Brojčin aktivno učestvuje u istraživanju nanostrukturnih materijala, posebno u razvoju i primeni numeričkih modela za analizu IC i Ramanovih, kao i modelovanju fotoluminescentnih (FL) spektara, koji omogućavaju sistematsko proučavanje strukturnih i elektronskih osobina velikog broja različitih nanomaterijala, u cilju razumevanja uticaja uslova sinteze na željene karakteristike i potencijalnu primenu. Dr Mirjana Grujić-Brojčin razvija je numeričke modele i softvere, koji su uspešno primenjeni na široku klasu nanostrukturnih materijala (nanoprahovi, kvantne tačke, kvantne žice, tanke slojevi i višeslojne strukture). U okviru ove oblasti ispitivani su TiO_2, CeO_2 i ZnO nanoprahovi, zatim SiO_x tanki filmovi, multislojevi ZnSe-SiO_x i tanki ZnSe filmovi.

Od 2009. godine, nastavljajući dalji razvoj i primenu numeričkih modela, dr Mirjana Grujić-Brojčin je učestvovala u proučavanju čistih i dopiranih TiO_2 nanoprahova sintetisanih sol-gel metodom i ZnO nanoprahova dobijenih mehaničkom aktivacijom komercijalnog ZnO praha, kao i ZnSe nanoslojeva.

1.1. Karakterizacija TiO_2 nanoprahova sintetisanih sol-gel metodom

Dr Mirjana Grujić-Brojčin je primenom MFO sprovela detaljnu analizu ponašanja najintenzivnijeg Ramanovog E_g moda anatas faze u nanoprahovima titanijum dioksida sintetisanim sol-gel metodom. Uočeno ponašanje E_g mod posledica je uticaja fononskog ograničenja, usled nanometarskih dimenzija kristalita (11-15 nm), ali i prisustva brukitne faze u uzorcima. Ova metoda karakterizacije omogućila je elementarnu identifikaciju faza i procenu veličine nanokristalita i sadržaja brukitne faze u uzorcima u zavisnosti od parametara sinteze, čime se došlo do optimizacije parametara procesa sinteze, kao što su pH vrednost

sredine prilikom prevođenja u gel, trajanje „starenja" gela, temperatura, brzina i vreme kalcinacije.

Dr Mirjana Grujić-Brojčin je primenom MFO ustanovila da je frekventni pomeraj i širenje E_g Raman moda posledica ne samo nanodimenzija anatas kristalita, već i neuređenosti indukovane prisustvom brukitne faze i La dopanta u uzorcima anatas nanoprahova dopiranih lantanovim jonima (La^{3+}) u osegu od 0 do 6 wt.%, sintetisanih takođe sol-gel metodom. Ovo je potvrdilo da dopiranje TiO_2 La^{3+} jonima znatno poboljšava faznu i nanostrukturnu stabilnost TiO_2 prahova na visokim temperaturama, čime se povećava efikasnost konverzije svetlosti, a dopiranje jonima La^{3+} doprinosi povećanju i stabilisanju temperature faznog prelaza anatasa.

Dr Mirjana Grujić-Brojčin je takođe pokazala da se MFO u kombinaciji sa modelom elastičnog kontinuuma koji opisuje akustičke fononske modove registrovane u nisko-frekventnom opsegu (<40 cm^{-1}) može iskoristiti za određivanje veličine nanočestica u nanoprahovima TiO_2 dopiranim La. Na ovaj način je pokazano i kako izbor koncentracije dopanta utiče na dobijene osobine nanočestica anatasa. Iz ove oblasti objavljena su 2 rada kategorije M22 i M23:

i M. J. Šćepanović, M. Grujić-Brojčin, Z. D. Dohčević-Mitrović, Z. V. Popović
"Characterization of Anatase TiO2 Nanopowder by Variable-Temperature Raman Spectroscopy"
Science of Sintering, 41 (2009) 67-73
M22

ii M. Šćepanović, S. Aškrabić, M. Grujić-Brojčin, A. Golubović, Z. Dohčević-Mitrović, A. Kremenović and Z.V. Popović
"Low-Frequency Raman Spectroscopy of Pure and La-Doped TiO_2 Nanopowders Synthesized by Sol-Gel Method"
Acta Physica Polonica A 116 (1) (2009) 94-102
M23

Dr Mirjana Grujić-Brojčin učestvovala je u ispitivanju nanoprahova titanijum dioksida, čistog i dopiranog vanadijumom, koji su takođe proizvedeni metodom sol-gel sinteze, gde proučavan uticaj uslova kalcinacije (temperature i trajanja) na njihove strukturne varijacije nanoprahova. Primenom Ramanove spektroskopije ustanovila je da temperatura i trajanje procesa kalcinacije imaju veliki uticaj na ponašanje najintenzivnijeg Ramanovog E_g moda, dok na nedopirane uzorke skoro da nemaju uticaj. Ovi rezultati pubikovani su u radu:

M. Šćepanović, S. Aškrabić, M. Grujić-Brojčin, A. Golubović, Z. Dohčević-Mitrović, B. Matović and Z.V. Popović
Raman study of vanadium-doped titania nanopowders synthesized by sol-gel method
International Journal Of Modern Physics B 24(6-7) (2010) 667-675
M23

Karakterizacija nanoprahova metodom spektroskopske elipsometije, kao i numeričko modelovanje eksperimentalnih rezultata bili su takođe predmet istraživanja dr Mirjane Grujić Brojčin.

Dr Grujić-Brojčin je primenom spektroskopske elipsometrije određivala dielektričnu funkciju laserski sintetisanih TiO_2 nanoprahova u energetskom opsegu od 1,5 do 6 eV na sobnoj temperaturi. Usaglašavanjem drugog izvoda eksperimentalno dobijenih spektara sa odgovarajućim analitičkim oblikom ovih funkcija, odredila je energije koje odgovaraju različitim međuzonskim elektronskim prelazima u anatas TiO_2 nanoprahovima i ustanovila da se energija koja se može pripisati indirektnom prelazu između valentne i provodne zone povećava sa smanjenjem veličine kristalita. Ovaj rezultat je publikovan u sledećem radu:

M. Šcepanović, M. Grujić-Brojčin, M. Mirić, Z. Dohčević-Mitrović and Z.V. Popović
"Optical Characterization of Laser-Synthesized Anatase TiO2 Nanopowders by Spectroscopic Ellipsometry and Photoluminescence Measurements"
Acta Physica Polonica A 116 (4) (2009) 603-606
M23

MFO takođe je modifikovan za primenu kod nanokristalnih agregata titaijum dioksida dopiranih gvožđem, gde je razmatran uticaj dopiranja gvožđem na pojavu tri faza titanijum dioksida u različizim uzorcima. Dr Grujić-Brojčin je primenila MFO na dve faze titanijum dioksida, anatas i rutil, i to 3D MFO na sferne nanočestice anatasa i 2D MFO na nanožice rutila, pokazavši tako da se povezivanjem rezultata Ramanove spektroskopije i XRPD može ostvariti kvalitetan uvid u morfologiju i heterogenost nanokristalnih agregata titanijum dioksida bogatih brukitom, sa malim količinama anatasa i rutila, čija pojava je korelisana sa koncentracijom dopanta Fe. Objavljen 1 rad kategorije M21:

A. Kremenović, M. Grujic Brojcin, A.-M. Welsch, P. Colomban
Heterogeneity in iron-doped titania flower-like nanocrystalline aggregates: Detection of brookite and anatase/rutile size-strain modeling
Journal of Applied Crystallography 46 (6) (2013) 1874-1876.
DOI:10.1107/S0021889813025363
M21

Zahvaljujući poznavanju velikog broja eksperimentalnih tehnika, numeričkih modela i optičkih karakteristika većeg broja oksidnih nanoprahova, dr Mirjana Grujić-Brojčin je dala značajan doprinos u objedinjavanju saznanja o uticaju metoda sinteze na optička svojstva oksidnih nanoprahova, posebno čistog i dopiranog titanijum dioksida u anatas fazi. Objavljena su 3 pregledna rada u međunarodnim časopisima, od kojih 2 po pozivu, u kojima se detaljno opisuju različiti aspekti primene MFO na Ramanove spektre oksidnih nanoprahova.

i M. Grujić-Brojčin, M.J. Šćepanović, Z.D. Dohcević-Mitrović and Z.V. Popović
"Use of Phonon Confinement Model in Simulation of Raman Spectra of Nanostructured Materials"
Acta Physica Polonica A Vol. 116(1) (2009) 51-54
M23

ii Z.V. Popović, Z. Dohčević-Mitrović, M. Šćepanović, M. Grujić-Brojčin and S. Aškrabić
"Raman scattering on nanomaterials and nanostructures"
Annalen Der Physik 523(1-2) (2011) 62-74
M23

iii Maja Šćepanović, Mirjana Grujić-Brojčin, Zorana Dohčević-Mitrović, and Zoran V. Popović
Investigation of vibrational and electronic properties of oxide nanopowders by spectroscopic methods
Journal of Physics: Conference Series 253 (2010) 012015

Na osnovu višegodišnjih istraživanja optičkih svojstava oksidnih nanoprahova, kao i doktorske disertacije dr Mirjane Grujić Brojčin, nastala je i monografija " Optička svojstva nanomaterijala", čiji je koautor i dr Grujić-Brojčin. U ovoj monografiji su sažete tehnike optičke karakterizacije i numeričkog modelovanja, sad detaljnom razradom metodologije i ilustrativnim rezultatima. Ramanova i fotoluminescentna spektroskopija, infracrvena spektroskopija i spektroskopska elipsometrija i njihove primene u karakterizaciji čistih i dopiranih TiO_2 i CeO_2 nanoprahova, kao i mehanički aktiviranih ZnO nanoprahova, razmatrane su u korelaciji sa drugim metodama kao što su XRD, SEM, AFM, TEM, BET itd.

Z. D. Dohčević-Mitrović, M.J. Šćepanović, M. Grujić-Brojčin, Z. V. Popović

"Optička svojstva nanomaterijala"
Institut za fiziku, Akademska misao 2011.
M41

1.2. Karakterizacija ZnO nanoprahova

U cilju ispitivanja vrste sopstvenih defekata i primesa uvedenih tokom procesa mehaničke aktivacije, Dr Mirjana Grujić-Brojčin je primenom metoda Ramnove spektroskopije dala značajan doprinos analizi aktiviranih prahova ZnO i sinterovanih keramika dobijenih od njih termičkim tretmanom. Ramanova spektroskopija primenjena je za istraživanje strukturnih i stehiometrijskih promena kod aktiviranih ZnO prahova u zavisnosti od vremena aktivacije i izbora aparature. Crveni pomeraj i širenje Ramanovih modova prvog reda E_2^{high} i E_1(LO), karakterističnih za ZnO, kod aktiviranih prahova pripisano je povećanoj neuređenosti prouzrokovanoj mehaničkim mlevenjem, praćenom smanjenjem korelacione dužine. Ovakvo ponašanje uspešno je simulirala primenom MFO, modifikovanog tako da se uključi efekat anizotropije Brillouin-ove zone. Promene koncentracije defekata, procenjena primenom MFO i odnosa intenziteta karakterističnih modova E_1(LO) / E_2^{high}, ukazale su na kiseonične vakancije kao dominantne defekte. Smanjenje odnosa intenziteta najintenzivnijeg Ramanovog moda drugog reda i E_1(LO) moda prvog reda takođe se ponaša u skladu sa smanjenjem korelacione dužine u aktiviranim prahovima. Dodatni Raman modovi na ~510 i 550 cm^{-1} u spektrima aktiviranih prahova pripisani su vibracijama površinskih optičkih fonona, koje se javljaju na granicama zrna između ultrafinih nanokristalita i neuređene oblasti u ZnO nanokristalitima. Ove modove je dr Grujić-Brojčin uspešno simulirala preko dielektrične funkcije i poroznih svojstava aktiviranih prahova usled prisustva vakancija, što je ukazalo na povećanje koncentracije defekata sa vremenom aktivacije u vibro-mlinu. Povećanje vremena aktivacije u planetarnom mlinu dovelo je do izvesne relaksacije u prahovima, praćene smanjenjem koncentracije sopstvenih defekata, ali i pojavom uvedenih defekata usled kontaminacije u cirkonijumskim posudama za mlevenje.

Uticaj neuređenosti na optička i elektronska svojstva aktiviranih ZnO takođe je ispitivan metodama fotoluminescentne spektroskopije i spektroskopske elipsometrije. Predložena je izmenjena interpretacija rezonantnog pojačanja Ramanovog rasejanja prvog i drugog reda u visokoneuređenim ZnO nanoprahovima. Detaljna analiza rezonantnog Ramanovog efekta u ZnO izazvanog laserskim zračenjem energije manje od energetskog procepa dala je značajne informacije o elektronskim stanjima unutar energetskog procepa ZnO nanoprahova. Uočeno je sistematska zavisnost jačine elektron-fonon sparivanja od korelacione dužine koja zavisi od neuređenosti kristalne rešetke ZnO.

Najvažniji rezultati koji se odnose na karakterizaciju mehanički aktiviranih ZnO prahova i od njih dobijenih keramika objavljeni su u 2 rada kategorije M21:

i M. Šćepanović, M. Grujić-Brojčin, K. Vojisavljević, and T. Srećković
"Defect induced variation in vibrational and optoelectronic properties of nanocrystalline ZnO powders"
Journal of Applied Physics 109 (2011) 034313

ii M. Šćepanović, M. Grujić-Brojčin, K. Vojisavljević, S. Bernik and T. Srećković
"Raman study of structural disorder in ZnO nanopowders"
Journal of Raman Spectroscopy 41 (2010) 914–921

1.3 Karakterizaciju ZnSe nanoslojeva primenom spektroskopske elipsometrije

U okviru ovih istraživanja dr Mirjana Grujić-Brojčin bavila se modelovanjem elipsometrijskih spektara ZnSe nanoslojeva. Pokazanala je da se može postići dobro slaganje

eksperimentalnih i modelovanih elipsometrijskih spektara ako se ZnSe nanoslojevi tretiraju kao polikristalni materijal modelovan kao smeša poroznog kristalnog ZnSe i amorfnog ZnSe primenom Bruggeman-ovog modela efektivne sredine. Ovakva struktura slojeva je u potpunoj saglasnosti sa rezultatima dobijenim primenom mikroskopa na bazi atomskih sila, kao i merenjima Ramanovog rasejanja i optičke transmisije. Rezultati dobijeni primenom spektroskopske elipsometrije takođe ukazuju na povećanje udela amorfne faze pri smanjenju debljine ZnSe sloja, što potvrđuje i kvantitativno opisuje nalaze dobijene mikroskopom na bazi atomskih sila. Rezultati ovog istraživanja, koji pokazuju da SE može dati veoma korisne informacije o kristaličnosti i nanostrukturi poluprovodničkih tankih slojeva, objavljeni su u radu:

M. Ščepanović, M. Grujić-Brojčin, D. Nesheva, Z. Levi, I. Bineva and Z.V. Popović
"Characterization of ZnSe Nanolayers by Spectroscopic Ellipsometry"
Acta Physica Polonica A 116 (4) (2009) 708-711
M23

2. Modelovanje optičkih i poroznih svojstava nanostrukturnih oksida za fotokatalitičke primene

Dr Mirjana Grujić-Brojčin je dala značajan doprinos uspešnoj primeni Ramanove spektroskopije za karakterizaciju čistih i dopiranih nanoprahova titanijum dioksida sintetisanih sol-gel metodom, namenjenih za fotokatalitičke primene. Iz merenja Ramanovog rasejanja određene su dominantne faze u sintetisanim nanoprahovima, kao i dimenzije i naprezanja u anatas nanokristalitima primenom metode fononskog ograničenja. Ovi eksperimentalni rezultati, u skladu sa XRD rezultatima, pokazali su da su svi sintetisani TiO_2 uzorci nanokristalni, sa dominantnom anatas fazom i malim sadržajem brukita. Ramanova spektroskopija takođe je korišćena za detektovanje i određivanje specifičnih površinskih grupa (CH, OH grupe) značajnih za proces fotokatalize, uprkos tome što se u tom spektralnom regionu javlja intenzivna fotoluminescencija. Zapaženo je da je mod na ~3700 cm^{-1}, pripisan vibracijama slobodnih hidroksilnih grupa aktivnih u procesu fotokatalize, prisutan kod čistih i uzoraka dopiranih lantanom koji pokazuju najveću fotokatalitičku aktivnost.

Uticaj dopiranja na energetski procep i energije elektronskih prelaza dr Mirjana Grujić-Brojčin ispitivala je primenom spektroskopske elipsometrije. Analiza rezultata pokazala je postojanje direktnog elektronskog prelaza u svim sintetisanim TiO_2 nanoprahovima, kao i da širina direktnog energetskog procepa u prahovima dopiranim lantanom raste sa povećanjem koncentracije La dopanta u TiO_2 zbog prisustva lantanovog oksida La_2O_3. Za potrebe ove analize dr Mirjana Grujić-Brojčin razvila je originalni softver.

Posebno značajan doprinos dr Mirjane Grujić-Brojčin predstavljaju analize rezultata merenja poroznosti nanoprahova titanijum dioksida. Osim BET i BJH metode, koje su uobičajene u analizi poroznosti, dr Grujić-Brojčin je porozne strukture sintetisanih prahova analizirala primenom CPS (*Corrugated pore structure*) modela, za koji kreirala numerički model i razvila odgovarajući originalni softver. Na osnovu CPSM procenjivan tzv. faktor "vijugavosti" (*tortuosity factor*), koji daje informacije o povezanosti pora, odnosno opisuje transportnu dinamiku porozne sredine, čime posredno određuje vreme fotokatalitičke reakcije, veoma značajan parametar u analizi fotokatalitičke aktivnosti poroznih materijala. Treba napomenuti da se ovaj model i softver, koji se uspešno koriste za modelovanje

poroznih svojstava nanoprahova titanijum dioksida, mogu se koristiti i za druge porozne materijale.

Na osnovu ovih rezultata, poboljšana fotokatalitička svojstva čistih i dopiranih TiO_2 nanoprahova pripisana su manjoj dimenziji nanočestica, većoj specifilčnoj površini i zapremini pora, kao i većoj kompleksnosti porozne strukture. Prisustvo izolovanih (slobodnih) hidroksilnih grupa kao izuzetno aktivnih pozicija u materijalu, registrovano je u TiO_2 nanoprahovima sa niskim sadržajem La, koji pokazuju najveću aktivnost u degradaciji metoprolola. U ovoj studiji takođe je pokazano da primenom metode spektroskopske elipsometrije može biti određena vrsta elektronskog prelaza u TiO_2. Analiza ovih rezultata pokazuje postepeni rast energetskog procepa sa dopiranjem, što može biti pripisano modifikaciji površine nanočestica TiO_2, što je i potvrđeno STM-STS merenjima. Do sada su objavljena 3 rada kategorije M21.

i Grujić-Brojčin, M., Armaković, S., Tomić, N., Abramović, B., Golubović, A., Stojadinović, B., Kremenović, A., Babić, B., Dohčević-Mitrović, Z., Šćepanović, M.
Surface modification of sol-gel synthesized TiO2 nanoparticles induced by La-doping
Materials Characterization 88 (2014) 30-41.

ii A. Golubović, B. Abramović, M. Šćepanović, M. Grujić-Brojčin, S. Armaković, I. Veljković, B. Babić, Z. Dohčević-Mitrović, and Z. V. Popović
"Improved efficiency of sol-gel synthesized mesoporous anatase nanopowders in photocatalytic degradation of metoprolol"
Materials Research Bulletin 48 (4) (2013) 1363-1371.

iii M. Šćepanović, B. Abramović, A. Golubović, S. Kler, M. Grujić-Brojčin, Z. Dohčević-Mitrović, B. Babić, B. Matović, Z. V. Popović
"Photocatalytic degradation of metoprolol in water suspension of TiO2 nanopowders prepared using sol–gel route"
Journal of Sol-Gel Science and Technology 61 (2012) 390–402

3. Primena metoda optičke spektroskopije u zaštiti kulturnih dobara

Dr Mirjana Grujić-Brojčin započela je 2013 aktivnosti na primeni metoda optičke spektroskopije u oblasti proučavanja i zaštite kulturnih dobara u okviru bilateralnog projekta "Scientific and technological cooperation between Sapienza University of Rome and University of Belgrade in the area of Cultural Heritage" koji je Institut za fiziku potpisao sa Univerzitetom Sapienca u Rimu. U okviru ove aktivnosti, dr Grujić-Brojčin se bavi ispitivanjem bojenih površina sa antičkih fresaka pronađenih na lokalitetu Sirmium i keramičkih artefakata sa nalazišta Kale-Krševica, u saradnji sa kolegama iz Instituta za arheologiju SANU i Instituta za nuklearne nauke Vinča.

ELEMENTI ZA KVALITATIVNU OCENU NAUČNOG DOPRINOSA KANDIDATA I MINIMALNI KVANTITATIVNI USLOVI ZA IZBOR

1. Pokazatelji uspeha u naučnom radu

1.1. Recenzije u međunarodnim časopisima

Dr Mirjana Grujić-Brojčin bila je recenzent u više međunarodnim časopisima, među kojima su: Materials Chemistry and Physics, Journal of Optics, Processing and Application of Ceramics, Materials Science and Engineering B, physica status solidi.

2. Angažovanost u razvoju uslova za naučni rad, obrazovanju i formiranju naučnih kadrova

2.1. Doprinos razvoju nauke u zemlji

Dr Mirjana Grujić-Brojčin učestvovala 2011. godine je kao koautor u izradi naučne mnografije nacionalnog značaja "Optička svojstva nanomaterijala" (Z. Dohčević-Mitrović, M. Šćepanović, M. Grujić-Brojčin, Z. V. Popović). Ova monografija predstavlja prvu publikaciju iz ove oblasti na srpskom jeziku, čime značajno doprinosi obrazovanju mladih naučnika u našoj zemlji.

Ova monografija daje pregled eksperimentalnih metoda optičke spektroskopije (Ramanova, fotoluminescentna, infracrvena spektroskopija, spektroskopska elipsometrija) i njihove primene na različite nanostrukturne materijale (oksidne nanoprahove čistih i dopiranih TiO_2, CeO_2, zatim mehanički aktivirane ZnO nanoprahove itd.), kao i brojne metode koji se koriste za modelovanje vibracionih spektara ovih materijala.

Baveći se više godina razvojem i usavršavanjem numeričkih metoda vezanih za vibracionu spektroskopiju nanostrukturnih materijala, dr Mirjana Grujić-Brojčin dala je originalan doprinos ovom radu. Istraživanja dr Grujić-Brojčin koja obuhvataju modele fononske lokalizacije i aproksimacije efektivne sredine, koji predstavljaju nezamenljive tehnike za pravilnu interpretacije Ramanovih i infracrvenih spektara nanostrukturnih materijala, našla su istaknuto mesto u ovoj monografiji.

2.2. Međunarodna saradnja

Dr Mirjana Grujić-Brojčin aktivno učestvovala u 3 međunarodne saradnje:

i Bilateralni projekat "**Scientific and technological cooperation between Sapienza University of Rome and University of Belgrade in the area of Cultural Heritage**" koji je Institut za fiziku 2013. godine potpisao sa Univerzitetom Sapienca u Rimu. Dr Mirjana Grujić-Brojčin se u okviru ovog projekta bavi primenom Ramanove spektroskopije u oblasti proučavanja i zaštite kulturnih dobara, konkretno izučavanjem bojenih površina i keramika sa antičkih nalazišta na teritoriji Republike Srbije.

ii Bilateralni projekat "**Raman Scattering and Photoluminescence from Semiconductor Nanoparticles**", koji je sklopljen 2004. godine između Instituta za fiziku čvrstog stanja Bugarske akademije nauka i Centra za fiziku čvrstog stanja i nove materijale Instituta za fiziku (projekat se realizuje kroz Ugovor o naučnoj saradnji između Srpske akademije nauka i umetnosti (SANU) i Bugarske akademije nauka (BAS)). U okviru ovog projekta dr Mirjana Grujić-Brojčin bavi se numeričkim modelovanjem Ramanovih spektara.

iii 2009-2012. godine na projektu bilateralne saradnje **SCOPES** sa Institutom za fiziku polimera Federalnim tehničkim institutom Cirih (ETH Zurich) Švajcarska. U okviru ovog projekta bavi se Ramanovom spektroskopijom nanoprahova za fotokatalitičke primene i numeričkim simulacijama Ramanovih spektara i poroznih svojstava oksidnih nanoprahova

2.3. Organizacija naučnih skupova

Dr Mirjana Grujić-Brojčin je član organizacionog odbora Društva za keramičke materijale Srbije, koje je organizovalo dve **međunarodne konferencije**:

i Drugu konferenciju Društva za keramičke materijale Srbije, 5-7. juna 2013. godine u Beogradu

ii Prvu konferenciju Društva za keramičke materijale Srbije, 17-18. marta 2011. godine u Beogradu

3. Organizacija naučnog rada

3.1 Projekti potprojekti i zadaci

Od 2008. godine dr Mirjana Grujić-Brojčin angažovana je na sledećim projektima Ministarstva za prosvetu, nauku i tehnološki razvoj Republike Srbije:

i 2006-2010. godine projekat MNTR Srbije br. 141047B "Fizika niskodimenzionih i nanometarskih struktura i materijala", rukovodilac prof. dr Zoran V. Popović

ii od 2010. godine angažovana na projektu ON17032 "Fizika nanostrukturnih oksidnih materijala i jako korelisanih sistema", rukovodilac dr. Zorana Dohčević-Mitrović

iii od 2010. godine angažovana na projektu III45018 "Nanostrukturni multifunkcionalni materijali i nanokompoziti", rukovodilac prof. dr Zoran V. Popović

Međunarodni projekti:

iv 2006-2009. godine dr Mirjana Grujić-Brojčin učestvuje u međunarodnom projektu *Centre of Excellence for Optical Spectroscopy Applications (OPSA-026283) in Physics, Material Science and Environmental Protection***,** koji se finansira od strane Evropske zajednice u okviru FP6 programa (2006-2009) i svojim radom doprinosi uspešnoj realizaciji ovoga projekta;

v 2009-2012. godine na projektu bilateralne saradnje SCOPES sa Institutom za fiziku polimera Federalnim tehničkim institutom Cirih (ETH Zurich) Švajcarska. U okviru ovog projekta bavi se Ramanovom spektroskopijom nanoprahova za fotokatalitičke primene i numeričkim simulacijama Ramanovih spektara i poroznih svojstava oksidnih nanoprahova;

vi od 2013. godine u bilateralnoj saradnji "Scientific and technological cooperation between Sapienza University of Rome and University of Belgrade in the area of Cultural Heritage", sklopljenom između Instituta za fiziku Univerziteta u Beogadu i Univerziteta Sapienca u Rimu, Italija. Bavi se primenom Ramanove spektroskopije na antičke pigmente i keramike;

vii od 2004. godine učestvuje u bilateralnoj saradnji "*Raman Scattering and Photoluminescence from Semiconductor Nanoparticles*", koji je sklopljen između Instituta za fiziku čvrstog stanja Bugarske akademije nauka i Centra za fiziku čvrstog stanja i nove materijale Instituta za fiziku.

Inovacioni projekti:

vii. 2008-2009. godine inovacioni projekat „Proizvodnja nanoprahova čistog i dopiranog anatasa vrhunskog kvaliteta pomoću sol-gel tehnologije“ (rukovodilac dr Aleksandar Golubović)

viii 2012-2013. godine inovacioni projekat "Proizvodnja visokokvalitetnih TiO_2 nanoprahova efikasnih u fotokatalitičkoj razgradnji organskih zagađivača" (rukovodilac dipl. inž. Dejan Ćukalović)

4. Kvalitet naučnih rezultata

4.1. Parametri kvaliteta časopisa i citiranost kandidatovih radova

Od prethodnog izbora u zvanje dr Mirjana Grujić-Brojčin objavila je 13 radova u međunarodnim časopisima, od čega **6 radova M21** (u vrhunski međunarodni), **1 rad M22** (vodeći međunarodni) i **6 radova M23** (međunarodn sa ISI liste).

Publikovala je do sada ukupno preko 60 naučnih referenci, od čega 35 radova u međunarodnim časopisima sa ISI liste.

Na osnovu pretrage indeksnih baza Web of Science/Scopus, za period od 1997. do kraja marta 2014. godine naučni radovi koje je dr Mirjana Grujić-Brojčin objavila citirani su više od **290 puta u međunarodnim časopisima, od toga 240 puta ne računajući autocitate**.
H indeks 8.

Posebno treba istaći sledeće radove:

		Broj citata
i	Z. D. Dohčević-Mitrović, M. J. Šćepanović, M.U. Grujić-Brojčin, Z.V. Popović, S.B. Bošković, B. M. Matović, M.V. Zinkevich, F. Aldinger The size and strain effects on the Raman spectra of Ce1-xNdxO2-δ (0≤x≤0.25) nanopowders, Solid State Communications 137 (2006) 387–390	51
ii	Šćepanović, M., Grujić-Brojčin, M., Vojisavljević, K., Bernikc, S., Srećković, T. Raman study of structural disorder in ZnO nanopowders	46

(2010) Journal of Raman Spectroscopy, 41 (9), pp. 914-921.

iii M. Grujić-Brojčin, M. J. Šćepanović, Z. D. Dohčević-Mitrović, I. Hinić, B. Matovic, G. Stanišić, and Z. V. Popović
Infrared study of laser synthesized anatase TiO_2 nanopowders 30
Journal of Physics D: Applied Physics 38 (2005) 1415-1420

iv Šćepanović, M.J., Grujič-Brojčin, M.U., Dohčević-Mitrović, Z.D., Popović, Z.V.
Effects of confinement, strain and nonstoichiometry on Raman spectra of anatase TiO2 nanopowders 24
(2006) Materials Science Forum, 518, pp. 101-106.

v M. J. Šćepanović, M. Grujić-Brojčin, Z. D. Dohčević-Mitrović, Z. V. Popović
Temperature dependence of the lowest frequency E_g Raman mode in laser-synthesized anatase TiO2 nanopowder 22
Appl. Phys. A 86 (3) (2007) 365-371

4.2.Tabele naučne kompetentnosti kandidata

i) Ukupno

M21=	6x8	=48
M22=	1x5	= 5
M23=	9x3	=18
M51=	1x1.5	= 2
M41=	1x7	= 7
Ukupno		**80**

ii) Od izbora u zvanje viši naučni saradnik

Potreban broj bodova kandidata po kategorijama i ukupno			**Zbir bodova kandidata**
	Ukupno potrebno	**48**	**80**
Viši naučni saradnik	M10+M20+M31+M32+ +M33+M41+M42+M51≥	40	80
	M11+M12+M21+M22++M23+ +M24+M31+M32+M41+M42≥	28	73