

Defect-induced colossal thermopower in FeSb₂

Cedomir Petrovic

Condensed Matter Physics, Brookhaven National Laboratory

Abstract. Recent interest in thermoelectric energy conversion stimulates search for new materials with high thermoelectric performance [1-2]. A narrow distribution or a large peak in the electronic density of states close to the Fermi level is considered favorable for high thermopower [3-4]. Such peak could be induced by the resonant level dopants in semiconductors [5-6] or by the magnetic interaction between the local magnetic moment and itinerant electrons [7-8]. Some strongly correlated materials show significant enhanced thermopower and power factor [9-10]. In this talk I will discuss FeSb₂ [11-13], a correlated electron semiconductor similar to FeSi [14] that was found to host a record-high thermopower of up to 50 mV/K [15]. The mechanism of colossal thermopower in FeSb₂ is presently not understood and moreover there is a wide variety in its reported values. In my talk I show how atomic defects create in-gap states of Fe orbital character that carry high electronic diffusion thermopower whereas phonon drag acting on such states – when crystal is engineered to have high phonon mean free path – enhances thermopower to colossal values. This reveals a subtle interplay of phonon and electronic diffusion mechanisms and points to relevant physics and crystal chemistry that can be exploited in predictive thermoelectric materials design.

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2018 Fall Meeting

LAYERED, HYBRID AND BIOMATERIALS

H

Emerging layered functional materials and their characterization

In layered systems different electronic degrees freedom compete to result self organized textures with ranging scales. In such cases the functional properties are described by these defects. Thematic meetings are common, however, EMRS is an ideal platform to discuss different functional properties originated from their layered structural topology.

Scope:

Various metal oxides/chalcogenides/pnictides with layered structure exhibit interesting and useful functional properties including high temperature superconductivity and giant thermoelectric performance. In these cases, the structural topology is deeply related to strong fluctuations of valence state and local bond. The layered structure topology of the functional materials is important also due to the fact that electronic degrees of freedom in the layered structures have strongly fluctuating character and the phases with charge (or magnetic order), coexisting with metallic (or superconducting) states can provide an effective mechanism for non-conventional phenomena. On the applied side, layered structures permit to have tuning of properties through external parameters as doping/intercalation, pressure, strain, electric and magnetic fields. This is of key interest for developing new materials through 'control and manipulation' for desired properties. Here, the focus is to discuss recent advances in the layered functional materials including emerging superconductors in which inhomogeneous ground state playing important role. In particular quantitative characterization of these materials is a challenging task requiring space and time resolved experimental tools applied under extreme conditions (e.g. pressure, electric and magnetic fields). The symposium welcomes contributions based on theoretical, experimental and applied aspects of the physics, chemistry, materials science on the hot topics given below.

Hot topics to be covered by the symposium:

- Physics and chemistry of layered thermoelectric materials
- Defect chemistry of layered pnictides and chalcogenides
- Layered ferroelectrics and quantum paraelectrics
- Pressure induced phases in layered materials
- Intrinsic structure of layered functional materials
- Emerging layered functional materials

List of invited speakers:

- Neven Barisic, Vienna
- Sara Barja, San Sebastián
- Atsushi Fujimori, Tokyo
- Hidetoshi Fukuyama, Tokyo
- Alexei Gruverman, Lincoln
- Shintaro Ishiwata, Tokyo
- Jun Sung Kim, Pohang
- Kazutaka Kudo, Okayama
- Chul-Ho Lee, Tsukuba
- Morgan Trassin, Zurich
- Jouko Nieminen, Tampere
- Tetsuji Okuda, Kagoshima
- Eugenio Paris, Zurich
- Cedomir Petrovic, Brookhaven
- Wilfrid Prellier, Caen
- Valerio Scagnoli, Zurich
- Shik Shin, Tokyo
- Julia Stähler, Berlin
- Yoshihiko Takano, Tsukuba
- Taishi Takenobu, Nagoya
- Hidenori Takagi, Stuttgart
- Kensei Terashima, Okayama
- Di Yi, Stanford

START AT	SUBJECT	View All	NUM.
14:30	<p>Superconducting Order from Disorder in 2D Charge Density Wave Materials</p> <p>Authors : Cedomir Petrovic Affiliations : Condensed Matter Physics, Brookhaven National Laboratory</p> <p>Resume : Superconductivity and charge-density-wave (CDW) are traditionally viewed as Fermi surface instabilities due to electron-phonon coupling whereas arguments have been made both for their cooperation and competition [1-3]. In copper oxides dome of high superconducting T_c exists at a rather complex phase diagram where disorder and various forms of symmetry breaking orders are present, such as spin-density, CDW or nematic order [4]. In this talk I will discuss emergence of superconductivity from the standpoint of disorder in doped two-dimensional (2D) CDW conductors ZrTe₃ and 2H-TaSe₂-xSx [5-10]. Superconducting domes in these materials exist in the absence of magnetism and could be of interest as an example of non-magnetic limit of copper oxide phase diagram. This work offers new 2D van der Waals bonded bulk single crystals for atomic layer engineering and possible tuning of cooperative phenomena at the nanoscale [11-12]. References: [1] G. Grüner, Rev. Mod. Phys. 60, 1129 (1988), [2] T. Kiss et al., Nature Physics 3, 720 (2007), [3] S. V. Borisenko et al., Phys. Rev. Lett. 102, 166402 (2009), [4] E. Fradkin et al., Rev. Mod. Phys. 87, 457 (2015), [5] Xiangde Zhu et al., Phys. Rev. Lett. 106, 246404 (2011), [6] Hechang Lei et al., Europhys. Lett. 95, 17001 (2011), [7] Xiangde Zhu et al., Sci. Rep. 6, 26974 (2016), [8] Lijun Li et al., NPJ Quantum Materials 2, 11 (2017), [9] M. Hoesch et al., arXiv:1712.03379, [10] A. M. Ganose et al., arXiv:1712.06551, [11] Xiaxiang Xi et al., Phys. Rev. Lett. 117, 106801 (2016), [12] Xiaoxiang Xi et al., Nature Physics 12, 139 (2016),</p>		H.3.2
15:00	Superconductivity and polymorphism in hexagonal Pt-based pnictides		H.3.3
15:30	Superconductivity and its Enhancement under High Pressure in "F-free" Single Crystals of CeOBiS ₂		H.3.4
	Layered thermoelectrics and related systems : T. Katsufuji		
16:00	Hole-doping effect on the Néel state of delafossite CuCrO ₂		H.4.1
16:30	Rattling dynamics under a planar coordination without oversized cages		H.4.2
17:00	Thickness-Driven Metal-Insulator Transition in CaVO ₃ : A Resonant Inelastic X-ray Scattering Study		H.4.3
	Poster session : T. Mizokawa, C. Kim		
17:30	2D to 3D phase transition study for In ₄ Se ₃ layered semiconductor crystal intercalated by Ag		H.P.1

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Symposium FF01 : Beyond Graphene 2D Materials—Synthesis, Properties and Device Applications

2019-12-01

2019-12-02

2019-12-03

2019-12-04

2019-12-05

2019-12-06

2019-12-04

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FF01.11: Exciton Dynamics in 2D Materials

Session Chairs

Deep Jariwala

Su Ying Quek

Wednesday AM, December 04, 2019

Hynes, Level 3, Room 312

8:00 AM - FF01.11.01

Exciton Dynamics in Atomically Thin Transition Metal Dichalcogenides

[Samuel Brem](#)¹, Simon Ovesen¹, Ermin Malic¹

Chalmers University of Technology¹

[Show Abstract](#)

9:30 AM - FF01.11.06

Strongly Anisotropic Diffusion of Excitons in Layered ReS₂ Observed with Transient Absorption Microscopy

Nicolas Gauriot¹, Hope Bretscher¹, Jooyoung Sung¹, Akshay Rao¹

University of Cambridge¹

Show Abstract

9:45 AM - FF01.11.07

Directional Exciton Transport in a Monolayer WS₂–WSe₂ Lateral Heterostructure with a Wide Alloy Region

Masafumi Shimasaki¹, Naoki Wada², Zheng Liu³, Kana Kojima², Yasumitsu Miyata², Keisuke Shinokita¹, Taishi Nishihara¹, Kazunari Matsuda¹, Yuhei Miyauchi¹

Institute of Advanced Energy, Kyoto University¹, Tokyo Metropolitan University², National Institute of Advanced Industrial Science and Technology³

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10:00 AM - FF01.11

BREAK

FF01.12: 2D Magnets—Materials and Properties**Session Chairs**

Angela Hight Walker
Amber McCreary

Wednesday PM, December 04, 2019
Hynes, Level 3, Room 312

10:30 AM - FF01.12.01

Critical Behavior and Thickness-Dependent Magnetic Order in CrI₃

Cedomir Petrovic¹, Yu Liu¹, Lijun Wu¹, Xiao Tong¹, Lijun Wu¹, Yimei Zhu¹

Brookhaven National Laboratory¹

Hide Abstract

Two-dimensional (2D) materials with intrinsic ferromagnetism provide unique opportunity to engineer new functionalities in nano-spintronics. One such material is CrI_3 , a 2D Ising ferromagnet in monolayer with the Curie temperature (T_c) of 45 K [1]. Based on critical properties and scaling analysis, CrI_3 shows three-dimensional (3D) long-range magnetic coupling [2]. In systematic reduction of crystal thickness down to 50 nm bulk T_c of 61 K is gradually suppressed to 57 K, however, the satellite transition at $T^* = 45$ K is observed. The T^* is layer-independent and corresponds to T_c observed in the monolayer. The critical analysis around T_c reveals a crossover from 3D to 2D Ising ferromagnetism with mean field type interactions for microscale-thick crystals. This work shows that magnetic transition and critical properties can be continuously tuned on a mesoscale between monolayer and bulk crystals.

Acknowledgements

This work has been supported by the Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences as part of the Computation Material Science Program (Y.L. and C. P.) and by the U.S. DOE under Contract No. DE-SC0012704 (L. W. X. T., J. L. and Y.Z.).

References

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11:00 AM - FF01.12.02

The Relation between Magnetism and Optical Properties in Lamellar Transition Metal Phosphor Tri-Chalcogenides

Efrat Lifshitz¹, Adam Budniak¹, Esty Ritov¹, Faris Horani¹, Yaron Amouyal¹

Technion - Israel Institute of Technology¹

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11:15 AM - FF01.12.03

Room-Temperature Dilute Magnetic Semiconductor in V-Doped Monolayer WSe_2

Dinh Loc Duong^{1,2}, Seok Joon Yun¹, Manh Ha Doan², Kirandeep Singh¹, Thanh Luan Phan¹, Wooseon Choi², Young Kuk Kim³, Young-Min Kim^{1,2}, Young Hee Lee^{1,2,3}

Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS)¹, Department of Energy Science, Sungkyunkwan University², Department of Physics, Sungkyunkwan University³

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Bulletin of the American Physical Society**APS March Meeting 2012**

Volume 57, Number 1

Monday–Friday, February 27–March 2 2012; Boston, Massachusetts

Invited Speakers**Y. Ozyilmaz, Barbaros**

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MIT Dept. of Electrical Engineering and Computer Science

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Photon Science, SLAC National Accelerator Laboratory**Affleck, Ian**

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Underscreened Kondo Effect](#) Room: 253AB

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Session D27.00001 [The DOE SunShot Initiative: Science and Technology to enable](#)

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Bulletin of the American Physical Society

APS March Meeting 2012

Volume 57, Number 1

Monday–Friday, February 27–March 2 2012; Boston, Massachusetts

Session D22: Focus Session: Fe-based Superconductors - Crystal Growth, Structure, and Properties of $K_xFe_{2-y}Se_{2-z}$ Phases

2:30 PM–5:30 PM, Monday, February 27, 2012

Room: 254B

Sponsoring Units: DMP DCOMP

Chair: Nicholas Butch, Lawrence Livermore National Laboratory

Abstract ID: BAPS.2012.MAR.D22.1

Abstract: D22.00001 : Superconductivity in $K_xFe_{2-y}Se_{2-z}S_z^*$

2:30 PM–3:06 PM

[Preview Abstract](#)

[Abstract](#) ➔

Author:

Cedomir Petrovic

(Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory)

Single crystal alloys $K_xFe_{2-y}Se_{2-z}S_z$ offer valuable insight into the strength of electronic correlations in the normal state and structural characteristics associated with superconductivity. I will discuss the evolution of the superconducting and magnetic ground states as a function of sulfur concentration z and some noticeable changes in the average and local crystal structure associated with this [1–4]. Conductivity and magnetic properties coincide with stoichiometry changes and with particular local environment of Fe atoms on the two Fe sites in the crystal structure. The ratio of superconducting T_c and Fermi temperature T_F is also suppressed by sulfur doping, indicating the suppression of electronic correlations. The superconductivity persists with relatively high T_c even when electronic correlations in the normal state are greatly reduced. The results for $z = 0$ will be compared with other experimental techniques that probe nanoscale phase separation and degree of vacancy order [5–6]. It will be shown that local structure and population of particular Fe sites is rather important for obtaining the bulk superconducting phase. Superconducting volume fraction and homogeneity of superconducting phase is in direct competition with Fe vacancy order [7]. [1] Hechang Lei et al., Phys. Rev. Lett. 107, 137002 (2011) [2] Hechang Lei et al., Phys. Rev. B 83, 180503 (2011) [3] Kefeng Wang et al., Phys. Rev. B 84, 054526 (2011) [4] Kefeng Wang et al., Phys. Rev. B 84, 054526 (2011) [5] Z. Wang et al., Phys. Rev. B 83, 140505 (2011) [6] Y. J. Yan et al., arXiv:1104.4941 (2011) [7] Hyejin Ryu et al., arXiv:1111.2597.

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