

# CURRICULUM VITAE

**Ji Hoon Shim**

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## A. Education and Professional Experience

### 1. Education

*2000-2004* Ph.D. Physics, Pohang University of Science and Technology, Korea  
Advisor: Professor Byung Il Min  
Thesis Title: "Electronic and magnetic structures, Fermi surface nesting, and susceptibilities of itinerant magnetic system"

*1994-2000* B.S. Physics, Pohang University of Science and Technology, Korea  
(Including the mandatory military service)

### 2. Professional Experience

*2013-* Associate Professor at Chemistry & Division of Advanced Nuclear Engineering, Pohang University of Science and Technology

*2012-2013* Director of Institute of Theoretical and Computational Chemistry (WCU program, Korea)

*2009-2012* Assistant Professor at Chemistry, Pohang University of Science and Technology

*2006-2008* Postdoctoral researchers at Physics, Rutgers University

*2004-2005* Postdoctoral researchers at Physics, Pohang University of Science and Technology

## B. Awards and Honors

*11/2009* **TJ Park Science Fellowship**  
POSCO TJ Park Foundation, Korea

*02/2008* **Named as an Outstanding Scientist**  
Ministry of Science and Technology, Korea

*08/2007* **C.N. Yang Award**

	Association of Asia Pacific Physical Societies
05/2007	<b>Named as an Outstanding Scientist</b> Ministry of Science and Technology, Korea
01/2006	<b>Foreign post-doc fellowship</b> Korea Research Foundation, Korea

### C. Research Interest

Prof. Shim has developed the computational method combining the density function theory and dynamical mean field theory (DFT+DMFT) for description of strongly correlated electron system. Using this method it becomes available to describe the electronic structures of d- and f-electron systems such as transition metal, rare earth and actinide compounds. Due to a variety of low energy phenomena they can exhibit, and sensitivity of these phenomena to chemistry and structure, there is a strong need for the first-principles predictive understanding of these materials. Recently, he also developed and applied those methods for the description of molecular orbital system which behaves like artificial d- and f-electron systems.

#### a. Development of DFT+DMFT method for strongly correlated electron system.

He developed the DFT+DMFT method for strongly correlated electron phenomena which arises from partially occupied d or f orbitals in transition metal compounds, rare earth, and actinide compounds [1]. These systems are located at the border of localization-delocalization transition, which amplify the importance of correct treatment of electronic correlations. In this respect, the DFT+DMFT method is becoming the most promising approach to describe their physical/chemical properties, because DMFT can correctly describe both the localized (atomic) and the itinerant (metallic) behavior of electrons. Indeed, by applying the DFT+DMFT method to actinide compounds, he firstly reveals the origin of anomalous physical and chemical properties of Plutonium which is the most puzzling element of the actinide elements [1]. He showed that it arises from a mixture of different atomic valences, which cannot be treated in other standard electronic structure techniques. He also applied the same approach to CeIrIn<sub>5</sub> heavy fermion compound [2,3], which behaves at low temperature as a metal with strongly enhanced electronic mass. After his first realistic calculation on actinide and rare earth compounds, he has also worked on the correlated electronic structures of the transition metal compounds [4-6].

#### b. Theoretical studies on transport properties of various functional materials

He has applied the DFT-based methods to various functional materials such as thermoelectric materials [7-9], superconductors [4,10], and Dirac materials [5,6]. For quantitative description of electrical and thermal conductivities, he has developed and used the DFT+DMFT method, Boltzman transport equation, and molecular dynamics calculation. He and his collaborators developed new concept with Peirels distortion or charge density wave to suggest high efficient thermoelectric materials In-Se compound which has the maximum ZT value among existing n-type thermoelectric materials [7]. Also by using the band engineering, the improvement of thermoelectric efficiency has been predicted and it was confirmed by the experiment [8]. Recently, he also suggested new concept for designing high efficiency thermoelectric materials by using the mixing of layer [9]. He also studied the anomalous electrical conductivity shown in rare earth heavy fermion compounds [10]. By reproducing the temperature-dependent electronic structures of Ce-based heavy fermion, he could

reveal the mechanism of temperature evolution of heavy fermion. His works on transport properties show the possibility of designing advanced functional materials from computational chemistry.

### c. Selected Publications

- (1) “Fluctuating valence in a correlated solid and the anomalous properties of delta-plutonium” J. H. Shim, K. Haule, G. Kotliar, *Nature* **2007**, *446*, 513.
- (2) “Modelling the Localized to Itinerant Electronic Transition in the Heavy Fermion System CeIrIn<sub>5</sub>” J. H. Shim, K. Haule, G. Kotliar, *Science* **2007**, *318*, 1615.
- (3) “Controlling Superconductivity by Tunable Quantum Critical Points” Soonbeom Seo, E. Park, Eric Bauer, Filip Ronning, J. Kim, Ji Hoon Shim, Joe Thompson, and Tuson Park, *Nature Comm.* **2015** (in press).
- (4) “Orbital selective Fermi surface shifts and mechanism of high T<sub>c</sub> superconductivity in correlated AFeAs (A=Li,Na)” Geunsik Lee, Hyo Seok Ji, Yeongkwan Kim, Changyoung Kim, Kristjan Haule, Gabriel Kotliar, Bumsung Lee, Seunghyun Khim, Kee Hoon Kim, Kwang S. Kim, Ki-Seok Kim, Ji Hoon Shim, *Phys. Rev. Lett.* **2012**, *109*, 177001.
- (5) “Anisotropic Dirac fermions in a Bi square net of SrMnBi<sub>2</sub>”, Joonbum Park, G. Lee, F. Wolff-Fabris, Y. Y. Koh, M. J. Eom, Y. K. Kim, M. A. Farhan, Y. J. Jo, C. Kim, J. H. Shim, J. S. Kim, *Phys. Rev. Lett.* **2011**, *107*, 126402.
- (6) “Valley-Polarized Interlayer Conduction of Anisotropic Dirac Fermions in SrMnBi<sub>2</sub>”, Y. J. Jo, Joonbum Park, G. Lee, Man Jin Eom, E. S. Choi, Ji Hoon Shim, W. Kang, Jun Sung Kim, *Phys. Rev. Lett.* **2014**, *113*, 156602.
- (7) “Peierls distortion as a route to high thermoelectric performance in In<sub>4</sub>Se<sub>3-x</sub> crystals”, J.-S. Rhyee, K. H. Lee, S. M. Lee, E. Cho, S. I. Kim, E. Lee, Y. S. Kwon, J. H. Shim, G. Kotliar, *Nature* **2009**, *459*, 965.
- (8) “Enhancement of thermoelectric figure-of-merit in a wide temperature range in In<sub>4</sub>Se<sub>3-x</sub>Cl<sub>0.03</sub> bulk crystals” Jong-Soo Rhyee, Kyunghan Ahn, Kyu Hyung Lee, Hyo Seok Ji, Ji-Hoon Shim, *Adv. Mater.* **2011**, *23*, 2191.
- (9) “Enhancing the thermoelectric properties of layered transition-metal dichalcogenides 2H-MQ<sub>2</sub> (M = Mo, W; Q = S, Se, Te) by layer mixing: Density functional investigation”, Changhoon Lee, Jisook Hong, Myung-Hwan Whangbo, Ji Hoon Shim, *Chem. Mater.* **2013**, *25*, 3745.
- (10) “Temperature-dependent Fermi surface evolution in heavy fermion CeIrIn<sub>5</sub>” Hong Chul Choi, B. I. Min, J. H. Shim, K. Haule, G. Kotliar, *Phys. Rev. Lett.* **2012**, *108*, 016402.

### D. Full List of Publications

#### Peer-Reviewed Original Research

#### - Since 2009 ~ Present: Independent contributions (Submitted and revision)

73. Changhoon Lee, Jisook Hong, Won-joon Son, Ji Hoon Shim \*, and Myung-Hwan Whangbo \*, “Magnetic structure of (C<sub>5</sub>H<sub>12</sub>N)CuBr<sub>3</sub>: Origin of the uniform Heisenberg chain behavior and the magnetic anisotropy of the Cu<sup>2+</sup> (S = 1/2) ions”, Submitted.

72. Changhoon Lee, Jisook Hong, Alessandro Stroppa, Myung-Hwan Whangbo \*, and Ji Hoon Shim

\*, “Organic-inorganic hybrid perovskites AB<sub>3</sub> (A = CH<sub>3</sub>NH<sub>3</sub>, NH<sub>2</sub>CHNH<sub>2</sub>; B = Sn, Pb) as potential thermoelectric materials: A density functional evaluation”, Submitted.

71. Jisook Hong, Changhoon Lee, Jin-Seong Park, and Ji Hoon Shim \*, “Control of valley degeneracy in MoS<sub>2</sub> by layer thickness and electric field”, Submitted.
70. J. D. Denlinger, J. W. Allen, J.-S. Kang, K. Sun, J.-W. Kim, Ji Hoon Shim, B. I. Min, Dae-Jeong Kim, and Z. Fisk, “Temperature Dependence of Linked Gap and Surface State Evolution in the Mixed Valent Topological Insulator SmB<sub>6</sub>”, Submitted.
69. Bo-Gyu Jang, Seung Ill Hyun, Moo Hwan Kim, Massoud Kaviani, and Ji Hoon Shim \*, “Physiochemical properties of uranium oxides from first principles”, Submitted.
68. Hyang Keun Yoo, Seung Il Hyun, Luca Moreschini, Young Jun Chang, Da Woon Jeong, Chang Hee Sohn, Yong Su Kim, Hyeong-Do Kim, Aaron Bostwick, Eli Rotenberg, Ji Hoon Shim, and Tae Won Noh \*, “Dimensional crossover of the electronic structure in LaNiO<sub>3</sub> ultrathin films”, Submitted.
67. Heejung Kim, J. N. Kim, J. H. Shim \*, and B. I. Min \*, “The role of van der Waals interaction in FeSe superconductor”, Submitted.

**- Since 2009 ~ Present: Independent contributions (Published articles)**

66. Jisook Hong, Jun-Won Rhim, Changyoung Kim, Seung Ryong Park \*, and Ji Hoon Shim \*, “Quantitative analysis on electric dipole energy in Rashba band splitting”, Scientific Reports, **2015**, Accepted (IF: 5.578)
65. Hoseok Heo, Ji Ho Sung, Soonyoung Cha, Bo-Gyu Jang, Joo-Youn Kim, Gangtae Jin, Donghun Lee, Ji-Hoon Ahn, Myoung Jae Lee, Ji Hoon Shim, Hyunyong Choi, and Moon-Ho Jo \*, “Interlayer Orientation Dependent Light Absorption and Emission in Monolayer Semiconductor Stacks”, Nature Communications, **2015**, 6, 7372 (IF: 11.47)
64. Thao P. Nguyen, Ji Hoon Shim\*, and Jin Yong Lee\*, “Density Functional Theory Studies of Hole Mobility in Picene and Pentacene Crystals”, The Journal of Physical Chemistry C, **2015**, 119, 11301–11310 (IF: 4.772)
63. Chan Su Jung, Han Sung Kim, Hyung Soon Im, Kidong Park, Jeunghye Park\*, Jae-Pyoung Ahn, Seung Jo Yoo, Jin-Gyu Kim, Jae Nyeong Kim, and Ji Hoon Shim \*, “In Situ Temperature-Dependent Transmission Electron Microscopy Studies of Pseudobinary mGeTe Bi<sub>2</sub>Te<sub>3</sub> Nanowires and First-Principles Calculations”, Nano Letters., **2015**, 15, 3923–3930 (IF: 13.592)
62. Heejung Kim, Chang-Jong Kang, Kyoo Kim, Ji Hoon Shim \*, and B. I. Min \*, “Phonon Softenings and the Charge Density Wave Instability in R<sub>2</sub>O<sub>2</sub>Sb (R: rare-earth elements)”, Physical Review B, **2015**, 91, 165130 (IF: 3.736)

61. Hyang Keun Yoo, Seung Ill Hyun, Luca Moreschini, Hyeong-Do Kim, Young Jun Chang, Chang Hee Sohn, Da Woon Jeong, Soobin Sinn, Yong Su Kim, Aaron Bostwick, Eli Rotenberg, Ji Hoon Shim, and Tae Won Noh \*, “Latent instabilities in metallic LaNiO<sub>3</sub> films by strain control of Fermi-surface topology”, *Scientific Reports*, **2015**, 5, 8746 (IF: 5.578)
60. S. Seo, E. Park, E. D. Bauer, F. Ronning, J. N. Kim, Ji Hoon Shim, J.D. Thompson, and Tuson Park \*, “Controlling superconductivity by tunable quantum critical points”, *Nature Communications*, **2015**, 6, 6433 (IF: 11.47)
59. Tae-Ho An, Young Soo Lim\*, Hyoung-Seuk Choi, Won-Seon Seo, Cheol-Hee Park, Gwi-Rang Kim, Chan Park, Chang Hoon Lee, and Ji Hoon Shim \*, “Point defect-assisted doping mechanism and related thermoelectric transport properties in Pb-doped BiCuOTe”, *Journal of Materials Chemistry A*, **2014**, 2, 19759-19764 (IF: 6.626)
58. Y. J. Jo, Joonbum Park, G. Lee, Man Jin Eom, E. S. Choi, Ji Hoon Shim, W. Kang, and Jun Sung Kim \*, “Valley-Polarized Interlayer Conduction of Anisotropic Dirac Fermions in SrMnBi<sub>2</sub>”, *Physical Review Letters*, **2014**, 113, 156602-156605 (IF: 7.512)
57. Changhoon Lee, Jisook Hong, Wang Ro Lee, Dae Yeon Kim, and Ji Hoon Shim \*, “Density functional theory investigation of the electronic structure and thermoelectric properties of layered MoS<sub>2</sub>, MoSe<sub>2</sub> and their mixed-layer compound”, *Journal of Solid State Chemistry*, **2014**, 211, 113-119 (IF: 2.133)
56. Changhoon Lee, Jinhee Kang, Jisook Hong, Ji Hoon Shim \*, and Myung-Hwan Whangbo \*, “Analysis of the Difference between the Pyroxenes LiFeSi<sub>2</sub>O<sub>6</sub> and LiFeGe<sub>2</sub>O<sub>6</sub> in Their Spin Order, Spin Orientation, and Ferrotoroidal Order”, *Chemistry of Materials*, **2014**, 26, 1745-1750 (IF: 8.354)
55. Muhammad A. Farhan, Geunsik Lee, and Ji Hoon Shim \*, “AEMnSb<sub>2</sub> (AE=Sr, Ba): a new class of Dirac materials”, *Journal of Physics- Condensed Matter*, **2014**, 26, 42201-42207 (IF: 2.346)
54. Jae Nyeong Kim, Changhoon Lee, and Ji Hoon Shim \*, “Chemical and Hydrostatic Pressure Effect on Charge Density Waves of SmNiC<sub>2</sub>”, *New Journal of Physics*, **2013**, 15, 123018 (IF: 3.558)
53. Minjae Kim, Hong Chul Choi, and Ji Hoon Shim \*, B. I. Min \*, “Correlated Electronic Structures and the Phase Diagram of Hydrocarbon-based Superconductors”, *New Journal of Physics*, **2013**, 15, 113030 (IF: 3.558)
52. Changhoon Lee, Jisook Hong, Myung-Hwan Whangbo \*, and Ji Hoon Shim \*, “Enhancing the thermoelectric properties of layered transition-metal dichalcogenides 2H-MQ<sub>2</sub> (M = Mo, W; Q = S, Se, Te) by layer mixing: Density functional investigation”, *Chemistry of Materials*, **2013**, 25, 3745-3752 (IF: 8.354)

51. Hong Chul Choi, K. Haule, G. Kotliar, B. I. Min \*, and J. H. Shim \*, “Observation of a kink during the formation of the Kondo resonance band in a heavy-fermion system”, *Physical Review B*, **2013**, 88, 125111 (IF: 3.736)
50. Hyungmin Ahn, Sungyeon Kim, Onnuri Kim, Ilyoung Choi, Chang-Hoon Lee, Ji Hoon Shim, and Moon Jeong Park \*, “Blue-emitting Self-assembled Polymer Electrolytes for Fast, Sensitive, Label-free Detection of Cu(II) ions in Aqueous Media”, *ACS Nano*, **2013**, 7, 6162-6169 (IF: 12.881)
49. Geunsik Lee, Muhammad A. Farhan, Jun Sung Kim, and Ji Hoon Shim \*, “Anisotropic Dirac electronic structure of AMnBi<sub>2</sub> (A=Sr,Ca)”, *Physical Review B*, **2013**, 87, 245104 (IF: 3.736)
48. D. W. Jeong, Hong Chul Choi, Choong H. Kim, Seo Hyoung Chang, C. H. Sohn, H. J. Park, T. D. Kang, Deok-Yong Cho, S. H. Baek, C. B. Eom, J. H. Shim, J. Yu, K. W. Kim, S. J. Moon, and T. W. Noh \*, “Temperature Evolution of Itinerant Ferromagnetism in SrRuO<sub>3</sub> Probed by Optical Spectroscopy”, *Physical Review Letters*, **2013**, 110, 247202 (IF: 7.512)
47. Hyo Seok Ji, Hyoungchul Kim, Changhoon Lee, Jong-Soo Rhyee, Moo Hwan Kim, Massoud Kaviany \*, and Ji Hoon Shim \*, “Vacancy-suppressed lattice conductivity of high-ZT In<sub>4</sub>Se<sub>3-x</sub>”, *Physical Review B*, **2013**, 87, 125111 (IF: 3.736)
46. Geunsik Lee, Hyo Seok Ji, Yeongkwan Kim, Changyoung Kim, Kristjan Haule, Gabriel Kotliar, Bumsung Lee, Seunghyun Khim, Kee Hoon Kim, Kwang S. Kim, Ki-Seok Kim, and Ji Hoon Shim \*, “Orbital selective Fermi surface shifts and mechanism of high T<sub>c</sub> superconductivity in correlated AFeAs (A=Li,Na)”, *Physical Review Letters*, **2012**, 109, 177001 (IF: 7.512)
45. Kyung Eun Lee, Byeong Hun Min, Jong-Soo Rhyee, Jae Nyeong Kim, Ji Hoon Shim , and Yong Seung Kwon \*, “Dimensional crossover of charge density wave and thermoelectric properties in CeTe<sub>2-x</sub>Sbx single crystals”, *Applied Physics Letters*, **2012**, 101, 143901 (IF: 3.302)
44. Hyo Seok Ji, Geunsik Lee, and Ji Hoon Shim \*, “Correlation Effect on the Electronic Structure of {Li,Na}FeAs”, *Progress in Superconductivity*, **2012**, 14, 11-16
43. Chang-Su Woo, Jin-Hong Lee, Kanghyun Chu, Byung-Kweon Jang, Yong-Bae Kim, Tae-Yeong Koo, Ping Yang, Yajun Qi, Zuhuang Chen, Lang Chen, Hong Chul Choi, Ji Hoon Shim, and Chan-Ho Yang \*, “Suppression of mixed-phase areas in highly elongated BiFeO<sub>3</sub> thin films on NdAlO<sub>3</sub> substrates”, *Physical Review B*, **2012**, 86, 054417 (IF: 3.736)
42. Erjun Kan, Xiaojun Wu, Changhoon Lee, Ji Hoon Shim, Ruifeng Lu, Chuanyun Xiao, and Kaiming Deng \*, “Two-dimensional organometallic porous sheets with possible high-temperature ferromagnetism”, *Nanoscale*, **2012**, 4, 5304-5307 (IF: 7.394)
41. J.-S. Lee, D. A. Arena, T. S. Santos, C. S. Nelson, S. I. Hyun, J. H. Shim, and C.-C. Kao \*

- “Controlling competing interactions at oxide interfaces: Enhanced anisotropy in  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  films via interface engineering”, *Physical Review B*, **2012**, 85, 235125 (IF: 3.736)
40. Hong Chul Choi, B. I. Min, J. H. Shim \*, K. Haule, and G. Kotliar , “Temperature-dependent Fermi surface evolution in heavy fermion  $\text{CeIrIn}_5$ ”, *Physical Review Letters*, **2012**, 108, 016402 (IF: 7.512)
39. Geunsik Lee and Ji Hoon Shim \*, “Electronic and Magnetic Structure of  $\{\text{Ca,Sr,Ba}\}\text{Fe}_2\text{As}_2$  : Dynamical Mean Field Theory Approach” , *Progress in Superconductivity*, **2011**, 13, 85-89
38. Joonbum Park, G. Lee, F. Wolff-Fabris, Y. Y. Koh, M. J. Eom, Y. K. Kim, M. A. Farhan, Y. J. Jo, C. Kim, J. H. Shim\*, and J. S. Kim \*, “Anisotropic Dirac fermions in a Bi square net of  $\text{SrMnBi}_2$ ”, *Physical Review Letters*, **2011**, 107, 126402 (IF: 7.512)
37. Hyo Seok Ji, Geunsik Lee, and Ji Hoon Shim \*, “Small anisotropy in iron-based superconductors induced by electron correlation”, *Physical Review B*, **2011**, 84, 054542 (IF: 3.736)
36. Jong-Soo Rhyee\*, Kyunghan Ahn, Kyu Hyung Lee, Hyo Seok Ji, and Ji-Hoon Shim, “Enhancement of thermoelectric figure-of-merit in a wide temperature range in  $\text{In}_4\text{Se}_3\text{-xCr}_{10.03}$  bulk crystals”, *Advanced Materials*, **2011**, 23, 2191 (IF: 17.493)
35. Minjae Kim, B. I. Min\*, Geunsik Lee, Hee Jae Kwon, Y. M. Rhee, and Ji Hoon Shim \*, “Density functional calculations of electronic structure and magnetic properties of the hydrocarbon  $\text{K}_3\text{picene}$  superconductor near the metal-insulator transition”, *Physical Review B*, **2011**, 83, 214510 (IF: 3.736)
34. Yoo Jang Song, Jin Soo Ghim, Jae Hyun Yoon, Kyu Joon Lee, Myung Hwa Jung, Hyo-Seok Ji, Ji Hoon Shim , Yunkyung Bang, and Yong Seung Kwon \*, “Small anisotropy of the lower critical fields and the s+ wave two-gap features in single-crystal  $\text{LiFeAs}$ ”, *EPL-Europhysics Letters*, **2011**, 94, 57008 (IF: 2.095)
33. Eun Cheol Lee, Young Cheol Choi, Woo Youn Kim, N. Jiten Singh, Sik Lee, Ji Hoon Shim , and Kwang S. Kim \*, “A Radical Polymer as Two-Dimensional Organic Half Metal”, *Chemistry-A European Journal*, **2010**, 16, 12141-12146 (IF: 5.731)
32. J. S. Kim, Seunghyun Khim, H. J. Kim, M. J. Eom, J. Law, R. K. Kremer, Ji Hoon Shim , and Kee Hoon Kim \*, “Electron-hole asymmetry in Co- and Mn-doped  $\text{SrFe}_2\text{As}_2$ ”, *Physical Review B*, **2010**, 82, 024510 (IF: 3.736)
31. J.-S. Rhyee, K. H. Lee, S. M. Lee\*, E. Cho, S. I. Kim, E. Lee, Y. S. Kwon, J. H. Shim , and G. Kotliar , “Peierls distortion as a route to high thermoelectric performance in  $\text{In}_4\text{Se}_3\text{-x}$  crystals”, *Nature*, **2009**, 459, 965-968 (IF: 41.456)
30. J.-S. Lee, E. Vescovo, C.-C. Kao, J.-M. Beaujour, A.D. Kent, H. Jang, J.-Y. Kim, J.-H. Park, and J.

H. Shim, “Role of the nonmagnetic Layer in determining the Lande g-factor in a spin-transfer system”, Physical Review B, **2009**, 80, 180403 (IF: 3.736)

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29. J. H. Shim\*, K. Haule, and G. Kotliar , “X-ray absorption branching ratio in actinides: LDA+DMFT approach”, EPL-Europhysics Letters, **2009**, 85, 17007 (IF: 2.095)
28. J. H. Shim\*, K. Haule, and G. Kotliar , “Density-functional calculations of the electronic structures and magnetism of the pnictide superconductors BaFeAs<sub>2</sub> and BaFeSb<sub>2</sub>”, Physical Review B, **2009**, 79, 060501 (IF: 3.736)
27. H. C. Choi, Amel Laref, J. H. Shim, S. K. Kwon, and B. I. Min \*, “Electronic structures and magnetic properties of RB<sub>4</sub> (R=Yb,Pr,Gd,Tb,Dy)”, Journal of Applied Physics, **2009**, 105, 07E107 (IF: 2.183)
26. J. H. Shim\*, K. Haule, S. Savrasov, and G. Kotliar , “Screening of magnetic moments in PuAm alloy : local density approximation and dynamical mean field theory study” , Physical Review Letters, **2008**, 101, 126403 (IF: 7.512)
25. K. Haule, J. H. Shim, and G. Kotliar , “Correlated Electronic Structure of LaO<sub>1-x</sub>F<sub>x</sub>FeAs”, Physical Review Letters, **2008**, 100, 266402 (IF: 7.512)
24. J. H. Shim\*, K. Haule, and G. Kotliar , “Modelling the Localized to Itinerant Electronic Transition in the Heavy Fermion System CeIrIn<sub>5</sub>”, Science, **2007**, 318, 1615 (IF: 33.611)
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21. H.C. Choi, J.H. Shim, S.K. Kwon, and B.I. Min , “Electronic structures and magnetic properties of layered compound RCrSb<sub>3</sub> (R=La, Yb)”, Journal of Applied Physics, **2007**, 101, 09G513 (IF: 2.183)
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19. H. C. Choi, J.H. Shim, and B.I. Min, “Electronic structures and magnetic properties of spinel ZnMn<sub>2</sub>O<sub>4</sub> under high pressure”, Physical Review B, **2006**, 74, 172103 (IF: 3.736)
18. J.-S. Kang, C.G. Olson, Y.S. Kwon, J.H. Shim, and B.I. Min , “Charge-density wave gap and



- dispersive Ce 4f states in CeTe<sub>2</sub> observed by photoemission” , Physical Review B, 2006, 74, 085115 (IF: 3.736)
17. B. I. Min, J. H. Shim, M. S. Park, Kyoo Kim, S. K. Kwon, and S. J. Youn , “Origin of the stabilized simple-cubic structure in polonium: Spin-orbit interaction versus Peierls instability” , Physical Review B, **2006**, 73, 132102 (IF: 3.736)
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  13. J. H. Shim, J.-S. Kang, and B. I. Min, “Electronic structures of RTe<sub>2</sub> (R=La, Ce): a clue to the pressure-induced superconductivity in CeTe<sub>1.82</sub>”, Physical Review Letters, **2004**, 93, 156406 (IF: 7.512)
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  11. J.-S. Kang, S. C. Wi, J. H. Kim, K. A. McEwen, C. G. Olson, J. H. Shim, and B. I. Min , “Electronic structures of UTSn (T=Ni, Pd) using photoemission spectroscopy”, Journal of Physics-Condensed Matter, **2004**, 16 (18) 3257-3269 (IF: 2.346)
  10. HS.C. Wi, J.-S. Kang, J.H. Kim, S.B. Cho, B.J. Kim, S. Yoon, B.J. Suh, S.W. Han, K.H. Kim, K.J. Kim, B.S. Kim, H.J. Song, H.J. Shin, J.H. Shim, and B.I.Min , “Photoemission study of Zn<sub>1-x</sub>CoxO as a possible DMS” ,Physica Status Solidi B-Basic Solid State Physics, **2004**, 241 (7), 1529-1532 (IF: 1.489)
  9. J. H. Shim and B. I. Min , “Electronic structures of layered compound LaCrSb<sub>3</sub> , Journal of Magnetism and Magnetic Materials”, **2004**, 272-276, E1565-E1566 (IF: 1.970)
  8. J.-S. Kang, J. H. Kim, YooJin Kim, WonSuk Jeon, Duk-Young Jung, S. W. Han, K. H. Kim, K. J. Kim, and B. S. Kim, J. H. Shim, and B. I. Min , “Investigation of the electronic structure of Mn<sub>12</sub> molecular magnet using synchrotron radiation” , Journal of Magnetism, **2003**, 8, 149-152 (IF: 3.736)

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7. J. -S. Kang, J. H. Kim, A. Sekiyama, S. Kasai, S. Suga, S. W. Han, K. H. Kim, E. J. Choi, T. Kimura, T. Muro, Y. Saitoh, C. G. Olson, J. H. Shim, and B. I. Min , “Resonant photoemission spectroscopy study of insulator-to-metal transition in Cr- and Ru-doped  $\text{Nd}_{1/2}\text{A}_{1/2}\text{Mn}_{1-y}\text{O}_3$  (A=Ca, Sr)”, *Physical Review B*, **2003**, 68, 012410 (IF: 3.736)
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5. J. -S. Kang, J. H. Kim, A. Sekiyama, S. Kasai, S. Suga, S. W. Han, K. H. Kim, T. Muro, Y. Saitoh, C. Hwang, C. G. Olson, B. J. Park, B. W. Lee, J. H. Shim, J. H. Park, and B. I. Min , “Bulk-sensitive photoemission spectroscopy of  $\text{A}_{2}\text{FeMoO}_{6}$  double perovskites (A=Sr, Ba)”, *Physical Review B*, **2002**, 66, 113105 (IF: 3.736)
4. J. -S. Kang, K. Nahm, C. K. Kim, C. G. Olson, J. Pelzl, J. H. Shim, and B. I. Min , “Valence-band photoemission study of  $\text{R}_3\text{S}_4$  (R=La, Ce)”, *Physical Review B*, **2002**, 66, 075108 (IF: 3.736)
3. J. H. Shim, S. K. Kwon, and B. I. Min , “Electronic structures of metallic antiperovskite compound  $\text{GaCMn}_3$ ”, *Physical Review B*, **2002**, 66, 020406 (IF: 3.736)
2. J. H. Shim, S. K. Kwon, and B. I. Min, “Electronic structures of antiperovskite superconductor  $\text{MgCNi}_3$  and related compounds”, *Journal of the Physical Society of Japan*, **2002**, 71 (Suppl.), 341 (IF: 1.585)
1. J. H. Shim, S. K. Kwon, and B. I. Min, “Electronic structures of antiperovskite superconductors:  $\text{MgXNi}_3$  (X = B, C, and N)”, *Physical Review B*, **2001**, 64 180510 (IF: 3.736)

#### **D. Invited Conference and Symposium Talks**

48. Control of Valley Degeneracy in  $\text{MoS}_2$  by Layer Thickness and Electric Field and Its Effect on Thermoelectric Properties  
The 8th Workshop for Emergent Materials Research, The 4rd Workshop of Max Planck POSTECH Center for Complex Phase Materials, Korea, 07/02/2015
47. Organic-inorganic hybrid perovskites as potential thermoelectric materials: A density functional evaluation  
Perovskite Optoelectronics Workshop, POSTECH, Korea, 06/19/2015
46. Phonon band engineering for thermoelectric materials design  
The 2nd Special TE Symposium in KIMM, Korea, 05/29/2015
45. Vacancy-Suppressed Lattice Thermal Conductivity of Low Dimensional  $\text{In}_4\text{Se}_{3-x}$   
2015 MRS Spring Meeting & Exhibit, USA, 04/09/2015

44. Electronic Structures of PAH-based Semiconductors and Superconductors  
Second China-Japan-Korea Tripartite Workshop on Theoretical and Computational Chemistry (CJK-WTCC-II), Japan, 01/21/2015
43. Thermoelectric Properties of GeTe/Bi<sub>2</sub>Te<sub>3</sub> Mixed Layer Compounds  
Electronic Materials and Nanotechnology for Green Environment 2014 (ENGE), Korea, 11/19/2014
42. Theoretical Study on Thermoelectric Efficiency of Organic-Inorganic Hybrid Perovskite  
THE 3rd International Symposium on Hybrid Materials and Processing (HYMAP 2014), NCRC for Hybrid Materials Solution, Korea, 11/11/2014
41. Anisotropic Dirac fermions in Bi square net system  
The 17th Asian Workshop on First-Principles Electronic Structure Calculations, Korea, 11/03/2014
40. The basic theory of the electronic structure: Tutorial on band theory  
The Korean Physical Society Fall Meetings, Korea, 10/22/2014
39. Topological Insulator phase of Americium Nitride: DFT+DMFT approach  
ALS USER MEETING (2014 ALS User Meeting Workshops), Lawrence Berkeley National Laboratory, USA, 10/08/2014
38. Theoretical design of thermoelectric materials using layer mixing  
The 5th International Symposium on Structure-Property Relationship in Solid State Materials (SPSSM-5), Qingdao University, China, 06/24/2014
37. Introduction to Band Theory  
The 2th IBS-Center for Correlated Electron Systems workshop, Korea, 06/19/2014
36. Tutorial on band theory!  
The 5th Condensed Matter Physics Summer School, Korea, 06/18/2014
35. Correlated Electronic Structures and Phase Diagram of Polycyclic Aromatic Hydrocarbon (PAH)-based Superconductors  
International Workshop of Computational Nano-Materials Design on Green Energy, Center of Asia Research & Education Network (CAREN), Japan, 06/02/2014
34. Competition between crystalline electric field and hybridization strength in YbRh<sub>2</sub>Si<sub>2</sub> under pressure  
The Fifth International Workshop on the DUAL NATURE OF F-ELECTRONS, SungKyunKwan University, Korea, 05/30/2014
33. First-principles design of thermoelectric materials by using layer mixing

- The Korean Institute of Metals and Materials Special Symposium on Thermoelectric Division, Korea, 02/06/2014
32. First-principles design of high-ZT thermoelectric materials  
The Korean Institute of Metals and Materials Fall Symposium on Fusion Materials and Science Division, Korea, 11/15/2013
  31. Enhancing the Thermoelectric Properties of Layered Transition-Metal Dichalcogenides  $2H-MQ_2$  ( $M = Mo, W; Q = S, Se, Te$ ) by Layer Mixing  
The Korean Physical Society Fall Meetings, Korea, 10/30/2013
  30. Observation of a kink during the formation of the Kondo resonance band in a heavy-fermion system  
2nd International Workshop on Convergence in Condensed Matter and Nano Physics, SungKyunKwan University, Korea, 10/07/2013
  29. Vacancy-suppressed lattice conductivity of high-ZT  $In_4Se_{3-x}$  compounds  
15th Asian Chemical Congress (15ACC), Singapore, 08/25/2013
  28. Correlated Electronic Structures of Polycyclic Aromatic Hydrocarbon (PAH)-based Superconductors  
The Sixth Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 6), Korea, 07/12/2013
  27. Precursor of the Kondo resonance band in the heavy fermion system  
Quantum materials symposium, APCTP, Korea, 01/29/2013
  26. Anisotropic Lattice Conductivity of high-ZT  $In_4Se_{3-x}$  with Se Vacancy  
EHSRC workshop 2012, University of Ulsan, 12/13/2012
  25. Correlation-Induced Non-Stoner-Type Itinerant Ferromagnetism of 3d Transition Metal Monomer Chains  
4<sup>th</sup> Symposium/Workshop on Computational Science (SWOCS4), POSTECH WCU&ITCC, Korea, 11/17/2012
  24. Orbital Selective Fermi Surface Shifts in Correlated AFeAs ( $A = Li, Na$ )  
The 11th A3 Foresight Program Joint Research on Novel Properties of Complex Oxides, China, 11/10/2012
  23. Competition between crystalline electric field and hybridization strength in  $YbRh_2Si_2$  under pressure  
The Fourth International Workshop on the Dual Nature of f-Electrons, Japan, 07/04/2012
  22. Anisotropic High-ZT  $In_4Se_{3-x}$  with Se Vacancy

- The 4th International Symposium on Structure-Property Relationship in Solid State Materials (SPSSM-4), France, 06/24/2012
21. Dual nature of f-electrons in solid: Lanthanides and Actinides  
The 8th Electronic Structure Calculation Workshop, KIAS, Korea, 06/20/2012
  20. Anisotropic Phonon Transport of  $\text{In}_4\text{Se}_{3-x}$  with Se Vacancy  
The Korean Society of Thermophysical Properties conference, Korea, 04/05/2012
  19. Electronic Structure and Magnetic Properties of the Hydrocarbon K3picene Superconductor near the Metal-Insulator Transition  
Korea-Japan Joint Symposium: Recent Trends of Polymer & Self-assembly Mat., University of Kitakyushu, Japan, 02/06/2012
  18. High Thermoelectric Figure-of-Merit in  $\text{In}_4\text{Se}_{3-x}$  Bulk Crystal  
3<sup>th</sup> Symposium/Workshop on Computational Science (SWOCS4), POSTECH WCU&ITCC, Korea, 11/09/2011
  17. Kinks during the formation of Kondo resonance state in heavy fermion ( $M = \text{Mo}, \text{W}; Q = \text{S}, \text{Se}, \text{Te}$ ) by Layer Mixing  
The Korean Physical Society Fall Meetings, Korea, 10/19/2011
  16. Temperature evolution of Fermi surface in heavy fermion system  $\text{CeIrIn}_5$   
Ultra Low Temperature Conference (ULT2011), KAIST, Korea, 08/19/2011
  15. Electron correlation in iron-based superconductors: Recent DMFT researches  
APCTP Summer Workshop on Frontiers in Electronic Quantum Matter, Korea, 06/29/2011
  14. Role of electron correlation in the small anisotropy of iron-based superconductors  
KIAS Workshop on Frontiers in condensed matter physics, Korea, 05/11/2011
  13. Hydrocarbon K3picene superconductor near the metal-insulator transition  
The Korean Physical Society Spring Meetings, Korea, 02/14/2011
  12. Electron correlation effect on the electronic & magnetic properties of iron pnictides  
Psi-k 2010 Conference, Germany, 09/14/2010
  11. Dynamical mean field theory and its combination with band theory  
The 2th Condensed Matter Physics Summer School, Korea, 07/07/2010
  10. Electronic structures of d- and f-orbital system: iron pnictide superconductors & plutonium compounds  
103th Korean Chemist Society Physical Chemistry Division Summer Symposium, Korea, 07/01/2010

9. Electronic structures and Magnetic Properties in PuSbxTe1-x: LDA+DMFT approach  
The 6<sup>th</sup> KIAS Electronic Structure Calculation Workshop, Korea, 06/22/2010
8. Magnetic phase diagram of Mn- and Co-doped SrFe2As2  
The Korean Physical Society Spring Meetings, Korea, 04/21/2010
7. Density-Functional Calculations of the Electronic Structures and Magnetism of the Pnictide Superconductors BaFeAs2 and BaFeSb2  
The Korean Superconductivity Society Meeting, Korea, 07/07/2009
6. Temperature evolution of Fermi surfaces in heavy fermion system CeCoIn5  
The 8<sup>th</sup> Asian Pacific Workshop on Novel Quantum Materials/2nd Workshop, Korea, 07/05/2009
5. Electronic structure of strongly correlated system: LDA+DMFT approach  
The 5<sup>th</sup> KIAS Electronic Structure Calculation Workshop, Korea, 06/18/2009
4. Materials Design from First Principles Calculation in Solids  
KCC physical chemistry branch meeting, Korea, 05/22/2009
3. Temperature evolution of Fermi surface in heavy fermion system Ce115  
The 12<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations, Beijing, China, 10/26-28/2009
2. Electronic structure of strongly correlated system: LDA+DMFT approach Symposium/Workshop on Computational Science (SWOCS4), POSTECH WCU&PBSRI, Korea, 11/22/2009
1. Electronic structures of  $R\text{Te}_{2-\delta}$  ( $R = \text{Ce, La}$ ), KIAS Workshop on Electronic Structure Calculations, Korea, 09/14/2004

## **E. Invited Lectures**

19. Evolution of heavy fermion under temperature and pressure changes in heavy fermion compounds and topological Kondo insulators, Department of Physics, University of Illinois at Chicago - UIC, 05/31/2015
18. Strongly Correlated Electron Systems: Dynamical Mean Field Theory Studies, Department of Physics Colloquium, Pohang University of Science and Technology, 05/13/2015
17. Evolution of heavy fermion under temperature and pressure changes in heavy fermion compounds and topological Kondo insulators, Carnegie Institution of Science, 12/18/2014
16. Evolution of heavy fermion under temperature and pressure changes in heavy fermion compounds and topological Kondo insulators, Rutgers University, 12/16/2014
15. Materials Design from First-Principles Calculations: Density Functional Theory Approach

- Department of Electrical Engineering, Pohang University of Science and Technology, 12/05/2014
14. Materials Design from First-Principles Calculations: DFT and DFT+DMFT approach, Department of Physics and Photon Science, Gwangju Institute of Science and technology, 10/15/2014
  13. Anisotropic Dirac fermions in Bi square net, University of California, Davis, 10/09/2014
  12. Introduction to Computational Materials Design, Pohang Idong High School, 04/23/2014
  11. Computational Design of Thermoelectric Materials, LG Chem, 03/23/2014
  10. Novel properties of Bi/Sb square net: Anisotropic Dirac Fermions and Metal-Insulator Transition, , Seoul National University, IBS, 01/04/2014
  9. Computational Approach of Advanced Materials: From Semiconductor to Nuclear Fuel, Daegu Gyeongbuk Institute of Science & Technology, 11/02/2012
  8. Computational Approach of Advanced Materials: From Semiconductor to Nuclear Fuel, University of Ulsan, 04/02/2012
  7. Temperature-dependent Fermi surface evolution in heavy fermion compounds, Seoul National University, 03/10/2012
  6. High Performance of Thermoelectric Figure-of-Merit in  $\text{In}_4\text{Se}_{3-x}$  Bulk Crystal, Korea Electrotechnology Research Institute, 12/06/2011
  5. Computer Simulations of Advanced Materials: From Semiconductors to Nuclear Fuel, Department of Physics seminar, Yonsei University, 03/23/2011
  4. Search for exotic materials: strongly correlated electron system, Department of Physics Seminar, SungKyunKwan University, 05/14/2010
  3. Search for exotic materials: strongly correlated electron system, Graduate School of EEWS Seminar, Korea Advanced Institute of Science and Technology, 04/28/2010
  2. Forming quasiparticles out of local moments, the case of heavy fermion  $\text{CeIrIn}_5$ , Department of Physics Seminar, Pohang University of Science and Technology, 08/22/2007
  1. Electronic structure of strongly correlated system: LDA+DMFT approach, Asia Pacific Center for Theoretical Physics (APCTP) Seminar, 09/24/2009

#### **F. Research Funding as a Principal Investigator (Excluding Intramural Funds)**

- \* The original Korean proposal titles are translated into English
- \*\* NRF stands for National Research Foundation of Korea
- \*\*\* Korean Won is converted to US Dollar at the rate of W1000 = \$1

**Korea Science and Engineering Foundation**

Research Duration	Project Title	Funds
12/2008-12/2013	Theoretical and Computational Science for Nano-Bio-Information Fusion	\$1,227,216
05/2010-04/2013	Theoretical design of superconducting materials	\$150,054
09/2010-08/2013	Study on the new quantum states in the dimensionality-controlled Ce-based compounds	\$180,000
09/2011-08/2015	Development of Thermoelectric Devices based on the Phonon-Engineered Materials	\$300,000
06/2012-05/2015	Quantum mechanical analysis in the improvement of thermal conductivity of U-based nuclear Fuel	\$235,000
09/2013-05/2016	Development of advanced thermoelectric materials using ab-initio calculation	\$153,270
01/2014-06/2016	The original technology of highly efficient organic/inorganic hybrid TE module	\$1,491,000
	<u>Subtotal:</u>	<u>\$3,736,540</u>

**Other Government Funding**

Research Duration	Project Title	Funds
01/2012-11/2014	Development of Molecular Dynamics Simulation of Thermal Properties (korea electrotechnology research institute)	\$101,818
03/2012-12/2014	Research on the design of thermoelectric material for high power generator (Agency for defense development)	\$499,000
02/2015-11/2015	Development of Thermal Properties Simulation Tools based on First-principles calculations (korea electrotechnology research institute)	\$31,818
	<u>Subtotal:</u>	<u>\$632,636</u>

**Industry Funding**

Research Duration	Project Title	Funds
10/2013-09/2014	Atomic-scale calculations of thermoelectric properties (LG Chem.)	\$50,000
	<u>Subtotal:</u>	<u>\$50,000</u>



Grand Total: \$4,419,176

## **G. Department and University, and Community Services**

### Services for the department

- Committee on Chemistry Undergraduate Program (2014 - 2015)

### Services for University

- POSTECH Dormitory Director (2012 - 2015)
- Dormitory Steering Committee (2012 - 2015)
- Committee on Student Counseling Center (2012 - 2015)
- Committee on Residential College Operation (2012 - 2015)
- Board of Directors on University Welfare Organization (2012 - 2015)
- Committee on Student Life (2012 - 2015)
- Committee on Sexual Harassment Counseling Office (2012 - 2015)

### Services for Science Communities

- Consultant on Daegu-Gyeongbuk Medical Cluster(2010-2012)
- Consultant on Workshop on First-Principles Calculation at KIAS (2014-2015)
- Editorial Board Member of Progress in Superconductivity and Cryogenics (2015)
- Research Council, Division of Condensed Matter Physics, Korean Physical Society (2015)

## **H. Professional Duties**

Reviewer for Journal of Physical Review Letters, Physical Review B, Advanced Materials, Applied Physics Letters, Proceedings of the National Academy of Sciences, Nano Letters, Nanoscale, New Journal of Physics, Dalton Transactions, Journal of Nuclear Materials, Journal of Solid State Chemistry, Philosophical Magazine, Physics Letters A, Journal of Alloys and Compounds, Journal of Nanostructure in Chemistry, Current Applied Physics, Journal of Electronic Materials, Bulletin of Korean Chemical Society, Progress in Superconductivity etc.

## **I. Conference Organization**

- Organization Committee, “The 5th Symposium/Workshop of Computational Sciences “, POSTECH, IES (2015)
- Organization Committee of a Session, "Korean Chemical Society Pioneering Symposium", Korean Physical Society (2014)
- Organization Co-chair of a Session, “International Workshop of Computational Nano-Materials Design on Green Energy”, Center of Asia Research & Education Network (2014)

- Organization Committee, “IES Workshop of Computational Science”, POSTECH, IES (2014)
- Organization Committee, “Mini-workshop on Dynamical Mean Field Theory”, POSTECH, IES/WCU (2013)
- Organization Committee, “Mini-workshop on Condensed Matter Theory”, POSTECH, IES (2012)
- Organization Committee, “13<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations”, POSTECH (2010)
- Organization Committee, “The 4th Symposium/Workshop of Computational Sciences”, POSTECH, ITCC (2012)
- Organization Committee, “The 3th Symposium/Workshop of Computational Sciences”, POSTECH, ITCC (2011)
- Organization Committee, “The 2th Symposium/Workshop of Computational Sciences”, POSTECH, ITCC (2010)
- Organization Committee, “The 1th Symposium/Workshop of Computational Sciences”, POSTECH, ITCC (2009)

## J. Professional Societies

- Materials Research Society(MRS)
- Korean Chemical Society (KCS)
- Korean Physical Society (KPS)
- Korean Superconductivity Society (KSS)

## K. Domestic Patents

### 1. Domestic Patents Filed

	Title	Inventors	Country	App. #
2	Thermoelectric device and method of fabricating the same	Jin-Seong Park, Lee Jung-Hoon, Ji Hoon Shim	Korea	10-2015-0050776
1	An electronic materials and manufacturing method of the same	Lim Jae Hong, Lee Kyu Hwan, Shim Ji Hoon, Lim Dong Chan, Song Young Sup, Heo Na Ri, ROH Sang Hyun	Korea	10-2015-0067358

### 2. Domestic Patents Registered

	Title	Inventors	Country	Reg. #
1	Thermoelectric materials optimized on thermoelectric property	Changhoon Lee, Jisook Hong, Dae Yeon Kim, Ji Hoon Shim	Korea	10-1469760-00-00