

## **Seong-Gon Kim, Ph.D.**

Department of Physics and Astronomy

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### ***Primary Research Areas***

- Computational physics; first-principles methods; Density Functional Theory; high-performance computing
- Electronic and structural properties of materials; molecular dynamics and structure optimization
- Nanoscale devices; molecular electronic devices; nanotubes and fullerenes; semiconductors; hydrogen catalysis
- Multiscale molecular dynamics simulations; Materials design of metal alloys and steels
- Magnetic materials; ferromagnetic-ferroelectric multiferroic materials
- Application of connectivity analysis to extremely large database and Internet search engines;

### ***Education***

- Ph.D. in Physics, 1994, Michigan State University, East Lansing, MI
- M.S. in Physics, 1988, Michigan State University, East Lansing, MI
- B.S. in Physics, 1986, Seoul National University, Seoul, Korea

### ***Professional Experiences***

- 2013 – present: Professor, Physics and Astronomy, Mississippi State University, Mississippi State, MS
- 2011 – present: Director, Center for Computational Sciences, High Performance Computing Collaboratory, Mississippi State University
- 2015 – present: Invitation Professor, Center for Integrated Nanostructure Physics, SungKyunKwan University, Korea
- 2015 – present: Visiting Professor, Department of Energy Science, SungKyunKwan University, Korea
- 2008 – 2013: Associate Professor, Physics and Astronomy, Mississippi State University, Mississippi State, MS
- 2008 – 2011: Associate Director, Center for Computational Sciences, High Performance Computing Collaboratory, Mississippi State University
- 2002 – 2008: Assistant Professor, Physics and Astronomy, Mississippi State University, Mississippi State, MS
- 2002 – 2008: Assistant Director, Center for Computational Sciences, High Performance Computing Collaboratory, Mississippi State University
- 2000 – 2001: Director of Technology, WiseNut, Inc., Santa Clara, CA

- 2000 – 2000: Research Assistant Professor, Vanderbilt University, Nashville, TN
- 1996 – 1999: Postdoctoral Associate, Naval Research Laboratory, Washington, DC
- 1994 – 1996: Research Associate, Center for Fundamental Materials Research, Michigan State University, East Lansing, MI

### ***Affiliations***

- American Physical Society
- Materials Research Society
- Korean Physical Society

### ***Professional Activities***

- Technical Advisory Board: Become, Inc., Mountain View, CA.
- Member: American Physical Society, Materials Research Society
- Grant Proposal Referee: National Science Foundation, American Chemical Society, U.S. Civilian Research and Development Foundation.
- Referee: Physical Review Letters, Physical Review B, Nano Research Letters, Journal of Alloys and Compounds, Surface Science, NanoLetter, Journal of Physics and Chemistry of Solids, Physica B.

### ***Grants***

1. 2002 – 2003, Ralph E. Powe Junior Faculty Enhancement Awards, “*First Principles Study of the Transport Phenomena in Molecular-scale Electronic Devices*,” Oak Ridge Associated Universities, PI, \$10,000.
2. 2002, Summer Research Grant, “*Molecular Electronic Devices and Spintronics*,” Mississippi State University, PI, \$7,167.
3. 2003 – 2007, “*Molecular Packing Software for ab initio crystal density predictions*,” Department of Defense, Common High Performance Computing Software Support Initiative (CHSSI) Project, Materials By Design Portfolio, co-PI, \$1,500,000.
4. 2004, “*First Principles Study of Atomic Potentials of Bi-Element Metallic Alloys*,” Center for Advanced Vehicular Systems, PI, \$22,000.
5. 2005, “*First Principles Study of Atomic Potentials of Bi-Element Metallic Alloys*,” Center for Advanced Vehicular Systems, PI, \$24,000.
6. 2005, “*First Principles Study of Interfaces and Defects Structures in Al-Mg Alloys*,” Center for Advanced Vehicular Systems, PI, \$49,000.
7. 2005, “*First Principles Study of Hydrogen Fuel Cell Catalysis*,” Center for Advanced Vehicular Systems, PI, \$77,500.
8. 2006 – 2008, “*Southern Regional Center for Lightweight Innovative Design*,” Department of Energy, co-PI, \$3,960,000.
9. 2007 – 2009, “*Center for Virtual Design and Manufacturing*,” Department of Energy, co-PI, \$2,376,000.

10. 2008—2010, “DOE Southern Regional Center for Lightweight Innovative Design Phase II – Task 6 Materials Design for Steel Alloys,” Department of Energy, PI, \$419,189.
11. 2008, “Workshop for Scientific Issues on Medical Applications of Micro/Nano Powder Injection Molding – Molding, Sintering, Modeling, and Commercial Application,” National Science Foundation, co-PI, \$32,000
12. 2008—2011, Henry Family Dean's Eminent Scholar Award Grant, Henry Family Foundation, PI, \$5,000.
13. 2009—2011, “SRCLID (Southern Regional Center for Lightweight Innovative Design) Phase III - Task 6 Materials Design for Steel Alloys,” Department of Energy, PI, \$348,726.
14. 2010—2011, “Tailoring Magnetic Properties of Hexagonal Ferrites for Army Applications,” Army Research Laboratory, PI, \$15,000.
15. 2010—2011, “Magnetic Materials for Nanoelectronics Research Group (MMNRG),” Cross-college Research Program, Office of Research and Economic Development, Mississippi State University, PI, \$3,200.
16. 2011—2012, “SRCLID (Southern Regional Center for Lightweight Innovative Design) Phase IV - Task 1: Multiscale Materials Models and Design Framework for Lightweight Alloys (Magnesium and Aluminum),” Department of Energy, co-PI, \$1,909,663.
17. 2011—2012, “SRCLID (Southern Regional Center for Lightweight Innovative Design) Phase IV - Task 2: Multiscale Materials Modeling and Characterization of Steel Alloys,” Department of Energy, co-PI, \$605,795.
18. 2011—2012, “Magnetic Materials for Nanoelectronics Research Group (MMNRG),” Cross-college Research Program, Office of Research and Economic Development, Mississippi State University, PI, \$2,000.
19. 2012—2014, “Rare Earth Free Permanent Magnets for Electrical Vehicle Motors and Wind Turbine Generators: Hexagonal Symmetry Based Materials Systems Mn-Bi and M-type Hexaferrite”, Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, co-PI, \$1,265,589.
20. 2012—2014, “Atomistic Simulation of metal matrix composites”, POSTECH, PI, \$59,285.
21. 2014—2015, “Manganese Based Permanent Magnet With 40 MGOe at 200°C: Task 11: Development of MnBi core and MnBi core-shell particles”, Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, co-PI, \$285,000.
22. 2016—2022, “Discovery of New Functional Electride through the Dimensional Control of Interstitial Electron Arrays”, Ministry of Science, ICT and Future Planning, Republic of Korea, PI, \$961,037.

### **Honors and Awards**

1. 1982—1986: Scholarships for academic achievements, Seoul National University.

2. 1988: Elected to membership in the ΦΚΦ honor's society for outstanding academic achievements, Michigan State University.
3. 2002: Ralph E. Powe Junior Faculty Enhancement Award.
4. 2005: Inducted to full membership of Sigma Xi Society.
5. 2007: Outstanding Researcher of the Year, Center for Advanced Vehicular Systems, Mississippi State University.
6. 2008: Certificate of Appreciation, Mississippi State University, Increasing Minority Access to Graduate Education (IMAGE) and the National Society of Black Engineers (NSBE).
7. 2008: 2008 Henry Family Dean's Eminent Scholar Award at Mississippi State University.
8. 2008: December/January's Researcher of the Month, College of Arts & Sciences, Mississippi State University.
9. 2009: Named as the delegate of Michigan State University to attend the inauguration of Dr. Mark Keenum as the 19<sup>th</sup> president of Mississippi State University.
10. 2010: 2010 StatePride Faculty Award, Mississippi State University.

### **Patents**

1. Seong-Gon Kim, Sudong Chung, Daeho Baek, *"Apparatus and method that categorize a collection of documents into a hierarchy of categories that are defined by the collection of documents ,"* United States Patent Application 2002/0169770 (Nov 14, 2002).
2. Yeogirl Yun, Seong-Gon Kim, Rohit Kaul, and Marcin Kadluczka, *"Systems and methods of retrieving topic specific information,"* United States Patent Application 2006/0074910 (Apr 6, 2006).
3. Seong-Gon Kim, Sudong Chung, Anurag Dod, Michael Kim, and Yeogirl Yun, *"Systems and methods of retrieving relevant information"* United States Patent 7,356,530 (Apr 8, 2008).
4. Rohit Kaul, Yeogirl Yun, and Seong-Gon Kim, *"Method for assigning quality scores to documents in a linked database,"* United States Patent 7,668,822 (Feb 23, 2010).
5. Rohit Kaul, Marcin Kadluczka, Yeogirl Yun, and Seong-Gon Kim, *"Method for assigning relative quality scores to a collection of linked documents,"* United States Patent 7,797,344 (Sep 14, 2010).

### **Publications**

1. S.G. Kim and P.M. Duxbury, *"Cracks and critical current,"* J. Appl. Phys. **70**, 3164–3170 (1991).
2. P.M. Duxbury, S.G. Kim and P.L. Leath, *"Size effect and statistics of fracture in random materials,"* Mat. Sci. and Eng. **A176**, 25–31 (1994).
3. Seong-Gon Kim and David Tomanek, *"Melting the fullerenes: A molecular dynamics*

- study*," Phys. Rev. Lett. **72**, 2418—2421 (1994).
4. P. Jund, S.G. Kim, D. Tomanek and J. Hetherington, "Stability and fragmentation of complex structures in Ferrofluids," Phys. Rev. Lett. **74**, 3049—3052 (1995).
  5. P. Jund, S.G. Kim, and C. Tsallis, "Crossover from extensive to nonextensive behavior driven by long-range interactions," Phys. Rev. B **52**, 50—53 (1995).
  6. A.G. Rinzler, J.H. Hafner, P. Nikolaev, L. Lou, S.G. Kim, D. Tomanek, P. Nordlander, D.T. Colbert, R.E. Smalley, "Unraveling Nanotubes: Field Emission from an Atomic Wire," Science **269**, 1550—1553 (1995).
  7. Andreas Thess, Roland Lee, Pavel Nikolaev, Hongjie Dai, Pierre Petit, Jerome Robert, Chinhui Xu, Young Hee Lee, Seong-Gon Kim, Andrew G. Rinzler, Daniel T. Colbert, Gustavo E. Scuseria, David Tomanek, John E. Fisher, Richard E. Smalley, "Crystalline Ropes of Metallic Carbon Nanotubes," Science **273**, 483—487 (1996).
  8. H. Gronbeck, D. Tomanek, S.G. Kim, and A. Rosen, "Does hydrogen pre-melt palladium clusters?" Chem. Phys. Lett. **264**, 39—43 (1997).
  9. K. German, H. Mizes, L. Belkhir, R. Lewis, S.G. Kim, and D. Tománek, Adhesion and chaining of magnetic particles, Proc. 20th annual meeting of the Adhesion Society in Hilton Head, SC, February 25, 1997.
  10. Seong-Gon Kim, Young Hee Lee, Peter Nordlander, David Tomanek, "Disintegration of finite carbon chains in electric fields," Chem. Phys. Lett. **264**, 345—350 (1997).
  11. H. Gronbeck, D. Tomanek, S.G. Kim, and A. Rosen, "Hydrogen induced melting of palladium clusters," Z PHYS D **40**, 469—471 (1997).
  12. David Tomanek, Seong-Gon Kim, Philippe Jund, Peter Borrmann, Heinrich Stamerjohanns, and Eberhard R. Hilf, "Self-assembly of magnetic nanostructures," Z PHYS D **40**, 539—541 (1997).
  13. Young Hee Lee, Seong-Gon Kim, David Tomanek, "Field-induced unraveling of carbon nanotubes," Chem. Phys. Lett. **265**, 667—672 (1997).
  14. Young Hee Lee, Seong-Gon Kim, David Tomanek, "Catalytic growth of single-wall carbon nanotubes: An *ab initio* study," Phys. Rev. Lett. **78**, 2393—2396 (1997).
  15. Young-Kyun Kwon, Young Hee Lee, Seong-Gon Kim, and David Tomanek, "Morphology and stability of growing multiwall carbon nanotubes," Phys. Rev. Lett. **79**, 2065—2068 (1997).
  16. Jan Westergren, Henrik Gronbeck, Seong-Gon Kim, and David Tomanek, "Noble gas temperature control of metal clusters: A molecular dynamics study," J. Chem. Phys. **107**, 3071—3079 (1997).
  17. D.J. Singh, I.I. Mazin, S.G. Kim and L. Nordstrom, "Computational studies of novel thermoelectric materials," Mat. Res. Soc. Sym. Proc. Vol. **478**, pp. 187-198 (1997).
  18. Seong-Gon Kim, I.I. Mazin and D.J. Singh, "First Principles Study of Zn-Sb Thermoelectrics," Phys. Rev. B **57**, 6199—6203 (1998).

19. P. Borrmann, H. Stamerjohanns, E.R. Hilf, P. Jund, S.G. Kim, and D. Tomanek, "Thermodynamics of finite magnetic two-isomer systems," *J. Chem. Phys.* **111**, 10689–10693 (1999).
20. M. Di Ventra, S. G. Kim, S. T. Pantelides, and N. D. Lang, "Temperature Effects on the Transport Properties of Molecules," *Phys. Rev. Lett.* **86**, 288–291 (2001).
21. Sanwu Wang, Massimiliano Di Ventra, S. G. Kim, and Sokrates T. Pantelides, "Atomic-Scale Dynamics of the Formation and Dissolution of Carbon Clusters in SiO<sub>2</sub>," *Phys. Rev. Lett.* **86**, 5946–5949 (2001).
22. S.T. Pantelides, R. Buczko, M. Di Ventra, S. Wang, S.-G. Kim, S.J. Pennycook, G. Duscher, L.C. Feldman, K. McDonald, R.K. Chanana, R.A. Weller, J.R. Williams, G.Y. Chung, C.C. Tin, T. Isaacs-Smith, "Bonding, defects, and defect dynamics in the SiC-SiO<sub>2</sub> system," in "Silicon Carbide – Materials, Processing and Devices", *Mat. Res. Soc. Symp. Proc.* Vol. **640**, pp. H.3.3.1–H.3.3.9, edited by A.K. Agarwal, J.A. Cooper, Jr., E. Janzen, M. Skowronski, Materials Research Society, Warrendale, Pennsylvania (2001).
23. S.G. Kim, S.C. Erwin, B.Z. Nosh, and L.J. Whitman, "Electronic versus geometric contrast in cross-sectional STM images of III-V semiconductor heterostructures," *Phys. Rev. B* **67**, 121306(R) [4 pages] (2003).
24. Sungho Kim and Seong-Gon Kim, "The Density Functional Theory Study Of The Adsorption Of Arsenic And Indium Atoms On (001) Surfaces Of GaSb Semiconductors," *High Performance Computing 2003*, 107–112 (2003).
25. Seong-Gon Kim, Sungho Kim, Jun Shen, B. Z. Nosh, S. C. Erwin, and L. J. Whitman, "Interface structures of III-V semiconductor heterostructures," *Int. J. Quant. Chem.* **95**, 561–571 (2003).
26. Seong-Gon Kim, Sungho Kim, and Jeffery Houze, "Recent Progress in Density Functional Theory and Its Applications," book chapter in "Recent Res. Devel. Quantum Chem." Vol. **5** (2006), pp. 15--53, ISBN:81-7895-169-X.
27. B. Jelinek, J. Houze, Sungho Kim, M. F. Horstemeyer, M. I. Baskes, Seong-Gon Kim, "Modified embedded-atom method interatomic potentials for the Mg-Al alloy system," *Phys. Rev. B* **75**, 054106 [9 pages] (2007)
28. J. Houze, Sungho Kim, Seong-Jin Park, Randall M. German, M. F. Horstemeyer, and Seong-Gon Kim, "Atomistic Simulations of Activated Sintering of Tungsten by Additives," *Advances in Powder Metallurgy & Particulate Materials 2007*, Part 1, 70–75 (2007).
29. Jeffery Houze, Sungho Kim, Seong-Gon Kim, S. C. Erwin and L. J. Whitman, "Structure of AlSb(001) and GaSb(001) surfaces under extreme Sb-rich conditions," *Phys. Rev. B* **76**, 205303 [6 pages] (2007).
30. Sungho Kim, Seong-Gon Kim, and S.C. Erwin, "Structure of the hydrogen double vacancy on Pd(111)," *Phy. Rev. B*, **76**, 214109 [5 pages] (2007).
31. J. Houze, Sungho Kim, Seong-Jin Park, Randall M. German, M. F. Horstemeyer, and Seong-Gon Kim, "The effect of Fe atoms on the adsorption of a W atom on W(100) surface," *J.*

- Appl. Phys. **103**, 106103 (2008).
32. Amitava Moitra, Sungho Kim, J. Houze, B. Jelinek, Seong-Jin Park, Randall M. German, M. F. Horstemeyer, and Seong-Gon Kim, "*Melting tungsten nanoparticles: a molecular dynamics study*," J. Phys. D: Appl. Phys., **41**, 185406 (2008).
  33. A. Moitra, S. Kim, S. G. Kim, S. J. Park, and R. M. German, "*Three Dimensional Atomistic Simulation of the Sintering and Shrinkage Behavior of Tungsten and Tungsten Alloys*," Proceedings of the 2008 International Conference on Tungsten, Refractory & Hardmaterials VII, Metal Powder Industry Federation, Princeton, NJ, 3-174 (2008).
  34. Rohit Kaul, Yeogirl Yun, and Seong-Gon Kim, "*Ranking billions of web pages using diodes*," Commun. ACM., **52** (8), 132-136 (2009).
  35. Seong-Gon Kim, M. F. Horstemeyer, M. I. Baskes, Masoud Rais-Rohani, Sungho Kim, B. Jelinek, J. Houze, Amitava Moitra, and Laalitha Liyanage, "*Semi-empirical Potential Methods for Atomistic Simulations of Metals and Their Construction Procedures*," J. Eng. Mater. Technol., **131** (4), 041210 [9 pages] (2009).
  36. Jeevan Jalli, Yang-Ki Hong, Seok Bae, Gavin S. Abo, Jae-Jin Lee, Jung-Chul Sur, Sung-Hoon Gee, Seong-Gon Kim, Steven C. Erwin and Amitava Moitra, "*Conversion of Nano-sized Spherical Magnetite to Spherical Barium Ferrite Nanoparticles for High Density Particulate Recording Media*," IEEE Trans. Magn. **45** (10), 3590-3593 (2009).
  37. Amber N. Yancey, Seong-Gon Kim, and John T. Foley, "*Visualizing Complicated Quantum Mechanical Behavior From Simple 2-D Potentials Using WebTOP*," International Journal of Modern Physics C, **20** (9), 1431-1441 (2009).
  38. Jinmu Choi, Seong-Gon Kim, Jiyeong Lee and Yun Soo Choi. "*Agent-Based Evacuation Simulation for Building Structure Evaluation*," GIScience & Remote Sensing, **46**(4), p. 1-18 (2009).
  39. Amitava Moitra, Sungho Kim, Seong-Gon Kim, Seong Jin Park, Randall German, and Mark Horstemeyer, "*Atomistic Scale Study on Effect of Crystalline Misalignment on Densification during Sintering Nano Scale Tungsten Powder*," Ceramic Transactions, **209**, 149–160 (2010).
  40. Jihoon Park, Yang-Ki Hong, Seok Bae, Jaejin Lee, Jeevan Jalli, Gavin S. Abo, Nick Neveu, Seong-Gon Kim, Chul-Jin Choi, and Jung-Gu Lee, "*Saturation magnetization and crystalline anisotropy calculations for MnAl permanent magnet*," J. Appl. Phys. **107**, 09A731 (2010).
  41. Amitava Moitra, Sungho Kim, Seong-Gon Kim, Seong Jin Park, Randall German, and Mark Horstemeyer, "*Investigation on sintering mechanism of nanoscale tungsten powder based on atomistic simulation*", Acta Materialia **58**, 3939–3951 (2010).
  42. Seong-Jin Park, S. Ahn, T.G. Kang, S.-T. Chung, Young-Sam Kwon, S.H. Chung, Seong-Gon Kim, A. Moitra, Randall M. German, "*A review of computer simulations in powder injection molding*," Inter. J. Powder Metallurgy, **46** (3), pp. 37-46 (2010).
  43. Jeevan Jalli, Yang-Ki Hong, Seok Bae, Jae-Jin Lee, Gavin S. Abo, Ji-Hoon Park, Alan M.

- Lane, Sung-Hoon Gee, Seong-Gon Kim, Steven C. Erwin, Moon J. Kim, and Terumitsu Tanaka, "Conversion of worm-shaped antiferromagnetic hematite to ferrimagnetic spherical barium-ferrite nanoparticles for particulate recording media", *IEEE Magn. Lett.* **1**, 4500204 (2010).
44. Jeevan Jalli, Yang-Ki Hong, Seok Bae, Jae-Jin Lee, Gavin S. Abo, Ji-Hoon Park, Byung-Chul Choi, Tim Mewes, Seong-Gon Kim, In-Tak Nam, and Terumitsu Tanaka, "Magnetic and microwave properties of ferrimagnetic Zr-substituted  $Ba_2Zn_2Fe_{12}O_{22}$  (Zn-Y) single crystals", *J. Appl. Phys.* **109**, 07A509 (2011).
  45. Sungho Kim, Seong-Gon Kim, Mark Horstemeyer, "Vanadium effects on a BCC iron sigma 3 grain boundary strength", *TMS Annual Meeting*, **2**, 617-619 (2011).
  46. Amitava Moitra, Seong-Gon Kim, and Mark F. Horstemeyer, "Structural and thermal properties of Calcium using a MEAM potential," *CALPHAD.* **35**, 262–268 (2011).
  47. Jeevan Jalli, Yang-Ki Hong, Seok Bae, Jae-Jin Lee, Gavin S. Abo, Tim Mewes, Byoung-Chul Choi, and Seong-Gon Kim, "Ferrimagnetic  $Sr_{1.5}Ba_{0.5}Zn_2Fe_{12}O_{22}$  ( $x = 0.5$ ) (Zn-Y) Single Crystal with Planar Anisotropy", *IEEE Magn. Lett.* **2**, 5000104 (2011).
  48. Jeevan Jalli, Yang-Ki Hong, Gavin S. Abo, Seok Bae, Jae-Jin Lee, Ji-Hoon Park, Byoung C. Choi, and Seong-Gon Kim, "MFM studies of domain patterns in bulk barium ferrite ( $BaFe_{12}O_{19}$ ) single crystals", *J. Magn. and Magn. Mater.* **323**, 2627–2631 (2011).
  49. Amitava Moitra, Sungho Kim, Seong-Jin Park, Seong-Gon Kim, and Mark F. Horstemeyer, "The Effect of Vanadium-Carbon Monolayer on the Adsorption. of Tungsten and Carbon Atoms on Tungsten-Carbide (0001) Surface", *Science of Sintering*, **43**, 153-159 (2011).
  50. Gavin S. Abo, Yang-Ki Hong, Jeevan Jalli, Jae-Jin Lee, Ji-Hoon Park, Seok Bae, Seong-Gon Kim, Byoung C. Choi, and Terumitsu Tanaka, "Shape Dependent Coercivity Simulation of a Spherical Barium Ferrite (S-BaFe) Particle with Uniaxial Anisotropy", *J. Magnetism* **17**, 1–5 (2012).
  51. B. Jelinek, S. Groh, A. Moitra, M. F. Horstemeyer, J. Houze, Seong-Gon Kim, G. J. Wagner, M. I. Baskes, "MEAM potentials for the Al, Si, Mg, Cu, and Fe alloys," *Phys. Rev. B* **85**, 245102 [18 pages] (2012).
  52. Yang-Ki Hong, Jihoon Park, Oleg N. Mryasov, Seong-Gon Kim, Sungho Kim, Jae-Jin Lee, Gavin S. Abo, Chul-Jin Choi, Junggoo Lee, "Magnetic properties of MnBi based alloys: First-principles calculations for MnBi-Co and MnBi-Co-Fe cases", *AIP Advances* **3**, 052137 (2013).
  53. Laalitha S.I. Liyanage, Sungho Kim, Yang-Ki Hong, Jihoon Park, S. C. Erwin, and Seong-Gon Kim, "Theory of magnetic enhancement in strontium hexaferrite through Zn-Sn pair substitution," *J. Magn. and Magn. Mater.* **348**, 75–81 (2013).
  54. Jihoon Park, Yang-Ki Hong, Seong-Gon Kim, Sungho Kim, Laalitha S.I. Liyanage, Jaejin Lee, Woncheol Lee, Gavin S. Abo, Kang-Heon Hur, Sung-Yong An, "Maximum energy product at elevated temperatures for hexagonal strontium ferrite ( $SrFe_{12}O_{19}$ ) magnet", *J.*

- Magn. and Magn. Mater. **355**, 1–6 (2013).
55. Laalitha Liyanage, Seong-Gon Kim, J. Houze, Sungho Kim, Mark A. Tschopp, M. I. Baskes, M. F. Horstemeyer, “Structural, elastic and thermal properties of cementite ( $Fe_3C$ ) calculated using Modified Embedded Atom Method,” *Phys Rev. B* **89**, 094102 (2014).
  56. Amitava Moitra, Seong-Gon Kim, and Mark F. Horstemeyer, “Solute effect on the  $\langle a + c \rangle$  dislocation nucleation mechanism in magnesium,” *Acta Mater.* **75**, 106–112 (2014).
  57. Jihoon Park, Yang-Ki Hong, Jaejin Lee, Woncheol Lee, Seong-Gon Kim, and Chul-Jin Choi, “Electronic Structure and Maximum Energy Product of  $MnBi$ ”, *Metals* **4**(3), 455–464 (2014).
  58. Amitava Moitra, Seong-Gon Kim, and Mark F. Horstemeyer, “Solute effect on basal and prismatic slip systems of Mg,” *Journal of Physics: Condensed Matter* **26**, 445004 (2014).
  59. Amitava Moitra, Sungho Kim, Seong-Gon Kim, S.C. Erwin, Yang-Ki Hong, Jihoon Park, “Defect formation energy and magnetic properties of aluminum-substituted M-type barium hexaferrite”, *Computational Condensed Matter* **1**, 45–50 (2014), doi: 10.1016/j.cocom.2014.11.001.
  60. Jihoon Park, Yang-Ki Hong, Seong-Gon Kim, Li Gao, and Jan-Ulrich Thiele, “Magnetic properties of Fe-Mn-Pt for heat assisted magnetic recording applications”, *J. Appl. Phys.* **117**, 053911 (2015), doi: 10.1063/1.4907570.
  61. Vivek Dixit, Chandani N. Nandadasa, Seong-Gon Kim, Sungho Kim, Jihoon Park, Yang-Ki Hong, Laalitha S. I. Liyanage, Amitava Moitra, “Site occupancy and magnetic properties of Al-substituted M-type strontium hexaferrite,” *J. Appl. Phys.* **117**, 243904 (2015).
  62. Vivek Dixit, Chandani N. Nandadasa, Seong-Gon Kim, Sungho Kim, Jihoon Park, Yang-Ki Hong, “Site preference and magnetic properties of Ga/In-substituted Strontium hexaferrite: an ab initio study,” *J. Appl. Phys.* **118**, 203908 (2015).
  63. Jihoon Park, Yang-Ki Hong, Hyun-Kyu Kim, Woncheol Lee, Chang-Dong Yeo, Seong-Gon Kim, Myung-Hwa Jung, Chul-Jin Choi, and Oleg N. Mryasov, “Electronic Structures of MnB Soft Magnet”, *AIP Advances* **6**, 055911 (2016).
  64. Jihoon Park, Yang-Ki Hong, Woncheol Lee, Seok Bae, Seong-Gon Kim, and Chul-Jin Choi, “Electronic Structures of Nanocrystalline  $Fe_{[90-x]}Cu_{[x]}Si_{[10-y]}B_{[y]}$ ”, *AIP Advances* **6**, 055915 (2016).
  65. Jihoon Park, Yang-Ki Hong, Chang-Dong Yeo, Seong-Gon Kim, David S. Kuo, Li Gao, and Jan-Ulrich Thiele, “Electronic Structure and Magnetic Properties of Mn Substituted Fe-Pt”, *IEEE Trans. Magn.* **52**, 3201904 (2016).
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  67. Park, Jong-Ho; Lee, Kimoon; Lee, Seung Yong; Nandadasa, Chandani; Kim, Sungho;

- Lee, Kyu Hyoung; Lee, Young Hee; Hosono, Hideo; Kim, Seong-Gon; Kim, Sung Wng, "Strong localization of anionic electrons at interlayer for electrical and magnetic anisotropy in two-dimensional Y<sub>2</sub>C electride", *J. Am. Chem. Soc.*, **139** (2), pp 615–618 (2017). (DOI: 10.1021/jacs.6b11950)
68. Jihoon Park, Yang-Ki Hong, Woncheol Lee, Seong-Gon Kim, Chuangbing Rong, Narayan Poudyal, J. Ping Liu, and Chul-Jin Choi, "A Simple Analytical Model for Magnetization and Coercivity of Hard/Soft Nanocomposite Magnets", *Scientific Reports*, vol. **7**, pp 4960 (2017) (DOI:10.1038/s41598-017-04632-6).
69. Vivek Dixit, Seong-Gon Kim, Jihoon Park, Yang-Ki Hong, "Effect of ionic substitutions on the magnetic properties of strontium hexaferrite: A first principles study," *AIP Advances* **7**, 115209 (2017). (DOI: 10.1063/1.4995309)
70. Park, Jong-Ho; Hwang, Jae-Yeol; Kyu Hyoung; Lee, Kim, Seong-Gon; Lee, Kimoon; Kim, Sung Wng, "Tuning the spin-alignment of interstitial electrons in two-dimensional Y<sub>2</sub>C electride via chemical pressure", *J. Am. Chem. Soc.*, **139** (48), pp 17277–17280 (2017). (DOI: 10.1021/jacs.7b10338)
71. Yujin Seong, Youngkyu Kim, Im Doo Jung, Sungho Kim, Seong-Gon Kim, See Jo Kim, Hak Jun Kim, Seong Jin Park, "Material Characterization of Single Crystalline Cu Subjected to High Strain Rates and High Temperatures for Multiscale Simulation", *Korean J. Met. Mater.*, Vol. **55**, No. 11 (2017), pp.760~767. (DOI: 10.3365/KJMM.2017.55.11.760)
72. K. P. Faseela, Ye Ji Kim, Seong-Gon Kim, Sung Wng Kim, and Seunghyun Baik, "Dramatically Enhanced Stability of Silver Passivated Dicalcium Nitride Electride: Ag-Ca<sub>2</sub>N", *Chemistry of Materials*, **30** (21), 7803-7812 (2018) (DOI: 10.1021/acs.chemmater.8b03202)
73. Laalitha S. I. Liyanage, Seong-Gon Kim, Jeff Houze, Sungho Kim, Mark A. Tschoop, Michael I. Baskes, Mark F. Horstemeyer, "From Electrons to Atoms: Designing an Interatomic Potential for Fe–C Alloys," Chapter 2 in "Integrated Computational Materials Engineering (ICME) for Metals: Concepts and Case Studies," ed. M. Horstemeyer, John Wiley & Sons (2018). (DOI:10.1002/9781119018377)
74. Seung Yong Lee, Jae-Yeol Hwang, Jongho Park, Chandani N. Nandadasa, Yonghak Kim, Kimoon Lee, Kyu Hyoung Lee, Yunwei Zhang, Yanming Ma, Hideo Hosono, Young Hee Lee, Seong-Gon Kim, and Sung Wng Kim, "Ferromagnetic quasi-atomic electrons in two-dimensional electride", under review, *Nature Comm.*
75. Vivek Dixit, Dinesh Thapa, Bipin Lamichhane, Chandani N. Nandadasa, Yang-Ki Hong, and Seong-Gon Kim, "Site preference and magnetic properties of Zn-Sn-substituted strontium hexaferrite", *J. Appl. Phys.* **125**, 173901 (2019) (DOI: 10.1063/1.5084762).
76. Se Hwang Kang, Yunwei Zhang, Yanming Ma, Chandani N. Nandadasa, Gyeongtak Han, Kyu Hyoung Lee, Sang-Ho Oh, Seong-Gon Kim, Young-Min Kim, and Sung Wng Kim, "Self-passivated dihafnium sulfide electride enabling a persistent electrocatalytic

reaction in water”, submitted to Nature Materials.

77. Sunghun Kim, Chan-young Lim, Jounghoon Hyun, Wonshik Kyung, Jonathan D. Denlinger, Seong-Gon Kim, Sung Wng Kim, and Yeong Kwan Kim, “Floating two-dimensional electron gas on the positively charged surface”, pre-print.
78. Chandani N. Nandadasa, SeHwang Kang, Jae-Yeol Hwang, Jongho Park, Gyeongtak Han, Kyu Hyoung Lee, Sang-Ho Oh, Young-Min Kim, Sung Wng Kim, Steven C. Erwin, and Seong-Gon Kim, “Real-space separation of conduction electrons at the metal-metal interface of hafniumsulfide electrified”, pre-print.
79. Yujin Seong, Youngkyu Kim, Im Doo Jung, See Jo Kim, Sungho Kim, Seong-Gon Kim, Hak Jun Kim; Seong Jin Park, "A Yield Criterion for Metals Subjected to High Strain Rates and High Temperatures for a Multiscale Simulation", under review for publication in Journal of Mechanical Science and Technology.

### *Presentations*

#### **Invited talks and colloquia**

1. Seong-Gon Kim, David Tomanek, Philippe Jund, Liang Lou, Peter Nordlander and Richard E. Smalley, “Morphology and stability of spot-welded carbon nanotubes,” Invited talk at the Annual Meeting of Korean Physical Society, DaeJeon, KOREA, October 27-28, 1995.
2. Seong-Gon Kim, Philippe Jund, and David Tomanek, “Formation of magnetic nanostructures,” Colloquium at Seoul National University, Seoul, KOREA, November 4, 1995.
3. Seong-Gon Kim, “Growth Mechanism and Disintegration Process of Carbon Nanotubes,” Colloquium at Wright Laboratory, Dayton, OH, July 30, 1996.
4. Seong-Gon Kim, “Computational Physics at the Frontier of Technology: Semiconductors and Molecular Electronic Devices,” Colloquium at Quantum Simulation Group, H Division, Lawrence Livermore National Laboratory, Livermore, CA, July 21, 2000.
5. Seong-Gon Kim, “Carbon Precipitation During Thin Film Oxidation of SiC,” Colloquium at Computational Materials Science Division, Lawrence Berkeley National Laboratory, Berkely, CA, November 19, 2001.
6. Seong-Gon Kim, “Transport Properties of Molecular Electronic Devices,” Colloquium at the Department of Materials Science, California Institute of Technology, Pasadena, CA, November 29, 2001.
7. Seong-Gon Kim, “Ordering Two Billion Webpages with A Random Walker,” Colloquium at the Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, July 17, 2002.
8. Seong-Gon Kim, “From Molecules to Mono-Molecular Electronic Devices,” Colloquium at the Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, July 24, 2002.

9. Seong-Gon Kim, "Carbon Precipitation During Thin Film Oxidation of SiC," Colloquium at the Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, July 31, 2002.
10. Seong-Gon Kim, "Advances in computational Molecular Electronics," Colloquium at Tokyo University, Tokyo, JAPAN, September 9, 2002.
11. Seong-Gon Kim, "Advances in computational Molecular Electronics," Colloquium at SungKyunKwan University, Suwon, KOREA, September 11, 2002.
12. Seong-Gon Kim, "Advances in Computational Molecular Electronics," Colloquium at Seoul National University, Seoul, KOREA, September 12, 2002.
13. Seong-Gon Kim, "Advances in computational Molecular Electronics," Colloquium at Korea Research Institute of Chemical Technology, Taejeon, KOREA, September 13, 2002.
14. Seong-Gon Kim, "Advances in computational Molecular Electronics," Colloquium at Pusan National University, Pusan, KOREA, September 14, 2002.
15. Seong-Gon Kim, "Ordering Two Billion Webpages with A Random Walker," Colloquium at the Department of Physics and Astronomy, Mississippi State University, Mississippi State, MS, November 18, 2002.
16. Seong-Gon Kim, "From Molecules to Mono-molecular Microprocessors," Colloquium at Physics Department, Brigham Young University, Provo, UT, January 28, 2003.
17. Seong-Gon Kim, "Density Functional Theory Study Of the Cross-Sectional STM Images of III-V Semiconductor Heterostructures and its Interface Formation Process," Plenary speaker, the 43rd Sanibel Symposium, St. Augustine, FL, February 22 - March 1, 2003.
18. Seong-Gon Kim, "Density Functional Theory Study Of the Interface Formation Process of III-V Semiconductor Heterostructures," Colloquium at Physics Department, Brigham Young University, Provo, UT, August 7, 2003.
19. Seong-Gon Kim, "From Molecules to Mono-molecular Microprocessors," Colloquium at Physics Department, University of Alabama, Tuscaloosa AL, November 12, 2003.
20. Seong-Gon Kim, "Quantum Delocalization of Hydrogen Atoms and Dissociative Hydrogen Adsorption on Metals," Colloquium at McGill University, Montreal, QB, Canada, Nov. 17, 2004.
21. Seong-Gon Kim, "Quantum Delocalization and Hydrogen Adsorption on Pd(111) Surfaces," Colloquium at Lawrence Berkeley National Laboratory, Berkeley, CA, Dec. 8, 2004.
22. Seong-Gon Kim, "Quantum violation of classical Langmuir adsorption kinetics," Colloquium at the Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, July 26, 2005.

23. Seong-Gon Kim, "Quantum wave nature of hydrogen on palladium," Invited speaker for the Atomistic Modeling And Simulation Seminars (AMASS) series at Massachusetts Institute of Technology, Cambridge, MA, August 22, 2005.
24. Seong-Gon Kim, "Ordering Eight Billion Webpages: A Physicist's Perspective," Invited seminar at the Department of Computer Science and Engineering, Mississippi State University, Mississippi State, MS, October 14, 2005.
25. Seong-Gon Kim, "DoD Planewave: A General Scalable Density Functional Code for Solids and Clusters," Invited talk at 2005 DoD High Performance Computing Modernization Program Workshop on Materials By Design at the Army Research Laboratory, Aberdeen Proving Ground, MD, December 7-8, 2005.
26. Seong Jin Park, Randall M. German, and Seong-Gon Kim, "CAVS Research Activities in Powder Metallurgy , Colloquium at Hanyang University," Seoul, KOREA, May 29, 2007.
27. Seong Jin Park, Randall M. German, and Seong-Gon Kim, "CAVS Research Activities in Powder Metallurgy," Seminar at Bestner, Inc., Seoul, KOREA, May 30, 2007.
28. Seong Jin Park, M.F. Horstemeyer, and Seong-Gon Kim, "Atomistic Simulations for Steel Alloy Design," Colloquium at POSTECH, Pohang, KOREA, June 4, 2007.
29. Seong Jin Park, M.F. Horstemeyer, and Seong-Gon Kim, "Atomistic Simulations for Steel Alloy Design," Seminar at Technical Research Laboratory of POSCO, Pohang, KOREA, June 5, 2007.
30. Seong-Gon Kim, "Ground-state structure of the hydrogen double vacancy on Pd(111)," Colloquium at the Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, July 20, 2007.
31. Seong-Gon Kim, "Materials Design for Steel Alloys by Multiscale Modeling", Keynote Speech at 45<sup>th</sup> Steel Technology Symposium, POSCO, Kwangyang, KOREA, July 17, 2008.
32. Seong-Gon Kim, Amitava Moitra, Sungho Kim, Seong Jin Park, Randall M. German, "*Atomistic Simulations of Nanoparticle Sintering*," Invited talk at Workshop on Medical Applications of Micro Powder Injection Molding, 2009 International Conference on Powder Injection Molding, March 2-5, Lake Buena Vista (Orlando), FL.
33. Seong Jin Park, S. Ahn, T. G. Kang, S.-T. Chung, Seong-Gon Kim, S. Kim, S. V. Atre, and R. M. German, "Granularity Issues in Computer Simulations Supporting Micro-PIM," Invited talk at Workshop on Medical Applications of Micro Powder Injection Molding, 2009 International Conference on Powder Injection Molding, March 2-5, Lake Buena Vista (Orlando), FL.
34. Seong-Gon Kim, "Ranking Billions of Web Pages Using Diodes: How Google works and how to beat it", Colloquium for Research Experience for Undergraduate (REU)

students, Mississippi State University, June 1, 2011.

35. Seong-Gon Kim, "Structural, elastic and thermal properties of cementite ( $\text{Fe}_3\text{C}$ ) from Modified Embedded Atom Method (MEAM) potential," Colloquium at Korea Aerospace Research Institute, Daejeon, KOREA, November 23, 2011.
36. Seong-Gon Kim, "Designing Better Alternatives to RareEarth Permanent Magnetic Materials: First principles approach based on Hexaferrites," Colloquium at SungKyunKwan University, Suwon, KOREA, November 24, 2011.
37. Seong-Gon Kim, "Structural, elastic and thermal properties of cementite ( $\text{Fe}_3\text{C}$ ) from Modified Embedded Atom Method (MEAM) potential," Colloquium at Pohang University of Science and Technology (*POSTECH*), Pohang, KOREA, November 29, 2011.
38. Seong-Gon Kim, "Designing Better Alternatives to RareEarth Permanent Magnetic Materials: First principles approach based on Hexaferrites," Colloquium at Pohang University of Science and Technology (*POSTECH*), Pohang, KOREA, November 30, 2011.
39. Seong-Gon Kim, "Ranking Billions of Web Pages Using Diodes: How Google works and how to beat it", Colloquium at Korea Maritime University, Busan, KOREA, December 1, 2011.
40. Seong-Gon Kim, "*Density Functional Theory Simulation of Sr-hexaferrite*," Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, Project Kickoff Meeting, Jan 17, 2012, Univ. of Alabama, Tuscaloosa, AL.
41. Seong-Gon Kim, "*Determination of magnetic properties of Sr-hexaferrite using GGA+U and HSE hybrid exchange-correlation functionals*," Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, Project Review Meeting, May 18, 2012, Univ. of California, San Diego, CA.
42. Seong-Gon Kim, "*Density Functional Theory Simulation of Magnetic Properties of Sr-hexaferrite*," Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, Project Kickoff Meeting, Oct 1, 2012, Univ. of Alabama, Tuscaloosa, AL.
43. Seong-Gon Kim, "*The effect of Zn-Sn Pair Substitution on the Magnetic Anisotropy of Sr-hexaferrite*," Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, Project Review Meeting, Jan 16, 2013, Chicago, Illinois.
44. Seong-Gon Kim, "*GGA+U simulation of the magnetic anisotropy of Sr-hexaferrite*," Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, Project Review Meeting, Jun 24, 2013, Detroit, MI.

45. Seong-Gon Kim, "*First principles calculations of the magnetic properties of MnBi-based magnets*," Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E), Rare Earth Alternatives in Critical Technologies for Energy (REACT) Program, Phase 2 Kickoff Meeting, Oct 15, 2013, Washington, DC.
46. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First principles approach based on Hexaferrites," Colloquium at Ulsan National Institute of Science and Technology (UNIST), Ulsan, KOREA, July 16, 2014.
47. Seong-Gon Kim, "*Theory of magnetic enhancement in strontium hexaferrite through Zn-Sn pair substitution*," Colloquium at Pohang University of Science and Technology (POSTECH), Pohang, KOREA, July 17, 2014.
48. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First principles approach based on Hexaferrites," Colloquium at Kyung Hee University, Seoul, KOREA, July 24, 2014.
49. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First principles approach based on Hexaferrites," Colloquium at Korea Institute of Ceramic Engineering & Technology, Seoul, KOREA, July 28, 2014.
50. Seong-Gon Kim, "Ranking Billions of Web Pages Using Diodes: How Google works and how to beat it," Colloquium at Korea Institute of Ceramic Engineering & Technology, Seoul, KOREA, July 28, 2014.
51. Jihoon Park, Yang-Ki Hong, Jaejin Lee, Woncheol Lee, Seong-Gon Kim, Chul-Jin Choi, "*Electronic Structure and Maximum Energy Product of Rare-earth Free Permanent Magnet (LTP-MnBi)*," Magnetic Materials for Energy Applications V, 2015 TMS Annual Meeting & Exhibition, Orlando, FL, March 15-19, 2015.
52. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First Principles Approach Based on Hexaferrites," Invited Lecture at Electronic Structure Calculation Workshop 2015, Korea Institute for Advanced Study, Seoul, KOREA, June 18-19, 2015.
53. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First Principles Approach Based on Hexaferrites," Colloquium at Pohang University of Science and Technology (POSTECH), Pohang, KOREA, July 15, 2015.
54. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First Principles Approach Based on Hexaferrites," Colloquium at Andong National University, Andong, KOREA, July 16, 2015.
55. Seong-Gon Kim, "Designing Better Alternatives to Rare-Earth Permanent Magnetic Materials: First Principles Approach Based on Hexaferrites," Colloquium at Korea Research Institute of Chemical Technology, Dajeon, KOREA, July 23, 2015.
56. Seong-Gon Kim, Chandani Nandadasa, Sungho Kim, Jongho Park, SeHwang Kang, Kimoon Lee, SungWng Kim, "Materials Properties of Y<sub>2</sub>C and Hf<sub>2</sub>S Electrides",

2016 Future Materials Discovery Project Workshop on New Functional Electrides, Busan, Korea, Jun. 28, 2016.

57. Seong-Gon Kim, Chandani Nandadasa, Sungho Kim, Jongho Park, Kimoon Lee, SungWng Kim, "Prediction of Materials Properties of Newly Designed Electrides", 2016 Future Materials Discovery Project Workshop on New Functional Electrides, Jeju, Korea, Nov. 6, 2016.
58. Seong-Gon Kim, "Electronic and magnetic properties of strong localization of anionic electrons in the interlayer of two-dimensional Y2C electride," Collaborative Conference on Materials Research (CCMR) 2017, Jeju, South Korea, June 26-30, 2017.
59. Seong-Gon Kim, Chandani Nandadasa, Seung-Yong Lee, Jongho Park, Kimoon Lee, SungWng Kim, "Materials Properties of Y2C and Gd2C Electrides", 2017 Future Materials Discovery Project Workshop on New Functional Electrides, Suwon, Korea, July 24, 2017.
60. Seong-Gon Kim, Chandani Nandadasa, Seung-Yong Lee, Jongho Park, Kimoon Lee, SungWng Kim, "Electric and magnetic properties Gd2C Electrides", 2017 Future Materials Discovery Project Workshop on New Functional Electrides, Suwon, Korea, Nov. 21, 2017.
61. Seong-Gon Kim, "Electronic and magnetic properties of strong localization of anionic electrons in the interlayer of two-dimensional Y2C electride", Colloquium at Korea Advanced Institute of Science and Technology (KAIST), Daejeon, KOREA, March 27, 2018.
62. Seong-Gon Kim, Chandani Nandadasa, Seung-Yong Lee, Jongho Park, Kimoon Lee, SungWng Kim, "Ferromagnetic quasi-atomic electrons in two-dimensional electride", 5th International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE 2018), Jeju, Korea, Nov. 11, 2018.

### **Contributed talks**

63. S.G. Kim and P.M. Duxbury, "Superflow Hotspots in Disordered Superconductors," APS March meeting in Saint Louise, MO, March 1989.
64. S.G. Kim and P.M. Duxbury, "Cracks and Critical Current," APS March meeting in Anaheim, CA, March 1990.
65. P.M. Duxbury and S.G. Kim, Scaling Theory and Simulations of Fracture in Disordered Media. P.M. Duxbury and S.C. Kim Proceedings of the ASME symposium on Damage Mechanics Dallas, Texas Nov, 1990
66. P.M. Duxbury and S.G. Kim, "Scaling Theory of Elasticity and Fracture in Disordered Networks," MRS Symp. Proc. 207, 179-195 (1991).
67. S.G. Kim and P.M. Duxbury, "Simulation of flux line lattice formation," APS March meeting in Indianapolis, IN, March 1991.
68. S.G. Kim and P.M. Duxbury, "Stability of Beam Networks," APS March meeting in Seattle, WA, March 1993.

69. Seong-Gon Kim and David Tomanek, "Melting of the carbon fullerenes," Midwest Solid State Theory Symposium at Wayne State University, Detroit, MI, October 1993.
70. Seong-Gon Kim and David Tomanek, "Melting the fullerenes: A molecular dynamics study," APS March meeting in Pittsburg, PA, March 1994.
71. Seong-Gon Kim and David Tomanek, "Melting of carbon fullerenes," Annual CFMR Symposium in E. Lansing, MI, April 1994.
72. Philippe Jund, Seong-Gon Kim, David Tomanek and Jack Hetherington, "Formation and Fragmentation of Complex Structures in Ferrofluids," APS March Meeting in San Jose, CA, March, 1995.
73. David Tomanek, Seong-Gon Kim, Philippe Jund, Liang Lou, Peter Nordlander and Richard E. Smalley, "Morphology and stability of open-ended carbon nanotubes," APS March Meeting in San Jose, CA, March, 1995.
74. Seong-Gon Kim, Philippe Jund, David Tomanek and Jack Hetherington, "Dynamics of Aggregation in Ferrofluids," APS March Meeting in San Jose, CA, March, 1995.
75. Seong-Gon Kim, Philippe Jund and David Tomanek, "Morphology and Stability of Open-Ended Carbon Nanotubes," Annual CFMR Symposium in E. Lansing, MI, April 1995.
76. S.G. Kim, P. Jund and D. Tomanek, "Morphology and stability of spot-welded carbon nanotubes," Gordon Conference on "Metal and Semiconductor Clusters", Colby-Sawyer College North, New London, NH, August 7-8, 1995.
77. P. Jund, S.G. Kim and D. Tomanek, "Formation of magnetic nanostructures," Gordon Conference on "Metal and Semiconductor Clusters", Colby-Sawyer College North, New London, NH, August 7-8, 1995.
78. Peter Borrmann, Seong-Gon Kim, Philippe Jund, Jian Chen, and David Tomanek, "Medication delivery by microspheres," Advanced Materials - Advanced Computing (AMAC) Symposium at Michigan State University, October 14, 1995.
79. David Tomanek, Seong-Gon Kim, Philippe Jund, Peter Borrmann, Heinrich Stamerjohanns, Eberhard R. Hilf, "Self-Assembly of Magnetic Nanostructures," APS March meeting in Saint Louise, MO, March 1996.
80. Peter Borrmann, Heinrich Stamerjohanns, Eberhard R. Hilf, Philippe Jund, Seong-Gon Kim, David Tomanek, "Thermodynamics of Finite Magnetic Two-Level Systems," APS March meeting in Saint Louise, MO, March 1996.
81. Henrik Gronbeck, Rosen Arne, David Tomanek, and Seong-Gon Kim, "Does Hydrogen Pre-Melt Palladium Clusters?", APS March meeting in Saint Louise, MO, March 1996.
82. Jian Chen, Seong-Gon Kim, and David Tomanek, "Melting and Metal-Insulator Transition in Sodium Clusters," APS March meeting in Saint Louise, MO, March 1996.

83. Seong-Gon Kim, David Tomanek, Philippe Jund, Liang Lou, A.G. Rinzler, J.H. Hafner, P. Nikolaev, Peter Nordlander, Daniel T. Colbert, and Richard E. Smalley, "Formation and Destruction of Multi-Walled Carbon Nanotubes," APS March meeting in Saint Louise, MO, March 1996.
84. David Tomanek, Seong-Gon Kim, Philippe Jund, Peter Borrmann, Heinrich Stamerjohanns, Eberhard R. Hilf, "Self-Assembly of Magnetic Nanostructures," ISSPIC 8 Conference in Copenhagen, DENMARK, July 1996.
85. Seong-Gon Kim, Young Hee Lee, and David Tomanek, "Formation and Disintegration of Carbon Nanotubes," ISSPIC 8 Conference in Copenhagen, DENMARK, July 1996.
86. Henrik Gronbeck, Rosen Arne, David Tomanek, and Seong-Gon Kim, "Hydrogen Induced Melting of Palladium Clusters," ISSPIC 8 Conference in Copenhagen, DENMARK, July 1996.
87. Peter Borrmann, Seong-Gon Kim, David Tomanek, and Philippe Jund, "Cracking Microspheres Using Magnetic Tops and External Fields," ISSPIC 8 Conference in Copenhagen, DENMARK, July 1996.
88. Seong-Gon Kim, I.I. Mazin, D.J. Singh, "First Principles Study of Zn-Sb Thermoelectrics," APS March meeting in Kansas City, MO, March 1997.
89. Young-Kyun Kwon, Young Hee Lee, Seong-Gon Kim, David Tomanek, "Equilibrium Structure of Multi-Wall Carbon Nanotubes," APS March meeting in Kansas City, MO, March 1997.
90. Seong-Gon Kim, R.W. Nunes, D.J. Singh, "First Principles Investigation of Surface Stacking Faults on Ru(0001)," APS March meeting in Los Angeles, CA, March 1998.
91. Seong-Gon Kim, S.A. Kajihara, D.J. Singh, C. Woodward, "DoD Planewave: A General Scalable Density Functional Code for Solids and Clusters," APS March meeting in Atlanta, GA, March 1999.
92. Seong-Gon Kim, Steve Erwin, Brett Noshko, and Lloyd Whitman, "First Principles Study of Cross-sectional Surface Structure of III-V Superlattices," APS March meeting in Minneapolis, MN, March 2000.
93. Sungho Kim and Seong-Gon Kim, "Density Functional Theory Study Of The Adsorption Of Arsenic And Indium Atoms On (001) Surfaces Of GaSb Semiconductors," APS March meeting, Austin, TX, March 2003.
94. Bohumir Jelinek, Seong-Gon Kim, Mark Horstemeyer, and Mike Baskes, "Ab-initio calculations for MEAM Potentials of Al, Si, Mg, H, O and Cu Alloys," SESAPS 2004, Oak Ridge, TN.
95. Jeff Houze, Mankang Mai, Sungho Kim and Seong-Gon Kim, "Density Functional Theory of GaSb(111) Surface Reconstruction," SESAPS 2004, Oak Ridge, TN.
96. Mankang Mai, Jeff Houze, Amber Benson, Sungho Kim and Seong-Gon Kim, "Ab-Initio Study of Solid Nitromethane," SESAPS 2004, Oak Ridge, TN.

97. Amber Benson, Sungho Kim and Seong-Gon Kim, "Structural Relaxation of Palladium (111) Surface with Dissociative Hydrogen Adsorption," SESAPS 2004, Oak Ridge, TN.
98. Sungho Kim, Seong-Gon Kim, and Steve Erwin, "Quantum Delocalization and Hydrogen Adsorption on Palladium," SESAPS 2004, Oak Ridge, TN.
99. Sungho Kim, Seong-Gon Kim, and Steve Erwin, "STM Image Simulation of quantum delocalization of hydrogen atoms and hydrogen adsorption on palladium," SESAPS 2004, Oak Ridge, TN.
100. Sungho Kim and Seong-Gon Kim, and Steve Erwin, "Quantum Delocalization and STM Image Simulation of Hydrogen Atoms Adsorbed on Pd(111) Surface," APS March meeting in Los Angeles, CA, March 2005.
101. Seong-Gon Kim, Sungho Kim, and Steve Erwin, "Quantum Delocalization and Hydrogen Adsorption on Pd (111) Surface," APS March meeting in Los Angeles, CA, March 2005.
102. Jeffery Houze, Sungho Kim, and Seong-Gon Kim, "Density functional theory study of GaSb(100) surface reconstruction," APS March meeting in Los Angeles, CA, March 2005.
103. Bohumir Jelinek, Seong-Gon Kim, Mark Horstemeyer, and Mike Baskes, "Ab-initio Calculations for MEAM Potential of Al, Si, Mg, H, O and Cu Alloys," APS March meeting in Los Angeles, CA, March 2005.
104. Sungho Kim, Seong-Gon Kim, and Steven C. Erwin, "Quantum Nature of Hydrogen on Metals: Ground-State Geometry of Vacancies," SESAPS 2005, Gainesville, FL, Nov. 10-12, 2005.
105. Seong-Gon Kim, Sungho Kim, and Steven C. Erwin, "Quantum Nature of Hydrogen on Metals: Dissociative Adsorption," SESAPS 2005, Gainesville, FL, Nov. 10-12, 2005.
106. Jeffery L. Houze, Sungho Kim, Seong-Gon Kim, and Steven C. Erwin, "GaSb(001) Surface Reconstruction: A First-principles Study," SESAPS 2005, Gainesville, FL, Nov. 10-12, 2005.
107. Bohumir Jelinek, Seong-Gon Kim, Mark Horstemeyer, and Mike Baskes, "MEAM Potentials for Al and Mg Alloys and Interfaces," SESAPS 2005, Gainesville, FL, Nov. 10-12, 2005.
108. Bohumir Jelinek, Jeffery Houze, Seong-Gon Kim, Mark Horstemeyer, and M. I. Baskes, "MEAM Potentials for Al-Mg Alloy: Application to Defects," APS 2006 March meeting, Baltimore, MD, Mar. 13-17, 2006.
109. Jeffery L. Houze, Sungho Kim, Seong-Gon Kim, and Steven C. Erwin, "Structure of III-Sb(001) Surfaces Under Extreme Sb-rich Conditions," APS 2006 March meeting, Baltimore, MD, Mar. 13-17, 2006.
110. Sungho Kim, Seong-Gon Kim, and Steven C. Erwin, "Quantum Nature of

- Hydrogen on Metals: Ground-State Geometry of Vacancies," APS 2006 March meeting, Baltimore, MD, Mar. 13-17, 2006.
111. Amitava Moitra, Sungho Kim, Seong-Gon Kim, Seong Jin Park, and Randall M. German, "Atomistic Simulations of Activated Sintering of Tungsten by Additives," PowderMet 2007, Denver CO.
  112. Sungho Kim, Seong-Gon Kim and Mark Horstemeyer, "First Principles Study of FCC-HCP Interface Dynamics Under Uniaxial Tension," APS 2006 SESAPS Meeting, Williamsburg, VA, Nov. 2006.
  113. Seong-Gon Kim, Jeffery L. Houze, Sungho Kim and Steven C. Erwin, "A First-principles Study of GaSb(001) Surface Reconstruction," APS 2006 SESAPS Meeting, Williamsburg, VA, Nov. 2006.
  114. Jeffery Houze, Bohumir Jelinek, and Seong-Gon Kim, "Molecular dynamics simulations of crack nucleation near nanoparticle inclusions," APS 2006 SESAPS Meeting, Williamsburg, VA, Nov. 2006.
  115. Bohumir Jelinek, Sungho Kim, Jeffrey Houze, Seong-Gon Kim, Mark Horstemeyer, and Mike Baskes, "Development and testing of MEAM Potentials for Al-Mg Alloys," APS 2006 SESAPS Meeting, Williamsburg, VA, Nov. 2006.
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