

# Curriculum Vitae

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## 1. ACADEMIC AND PROFESSIONAL HISTORY

- **A.B. in Physics, Harvard University, Cambridge, Massachusetts. 1989-1993.**
  - **D.E.A. degree in Statistical Physics and Non-linear Phenomena, Ecole Normale Supérieure de Lyon, Lyon, France. 1993-1994.**
  - **Ph.D. in Physics, MIT, Cambridge, Massachusetts. Student of Prof. Tomás Arias. 1994-2000.**
  - **Postdoctoral Researcher in Physics, University of California at Berkeley and Lawrence Berkeley National Laboratory, Berkeley, California. Worked in the group of Prof. Steven G. Louie. 2000-2003.**
  - **Assistant Professor, Department of Applied Physics and Department of Physics, Yale University, New Haven, Connecticut. 2003-2007**
  - **Associate Professor on term, Department of Applied Physics and Department of Physics, Yale University, New Haven, Connecticut. 2007-2011**
  - **Associate Professor with tenure, Department of Applied Physics and Department of Physics, Yale University, New Haven, Connecticut. 2011-2014**
  - **Professor with tenure, Department of Applied Physics, Department of Physics, and Department of Mechanical Engineering and Materials Science, Yale University, New Haven, Connecticut. 2015-present**
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## 2. FUNDING

Present funding

- IRG1 co-leader in CRISP (Center for Research on Interface Structures and Phenomena) which is Yale's NSF MRSEC (PI Charles Ahn, 09-/2011-08/2017, \$7,000,000 first year): NSF DMR-1119826. Previous Yale MRSEC (2005-2011) and current one support two graduate students and one postdoctoral fellow in Ismail-Beigi group.
- SI2-SSI: Collaborative Research: Scalable, Extensible, and Open Framework for Ground and Excited State Properties of Complex Systems, (PI Sohrab Ismail-Beigi, 9/12/2013-9/30/2018, \$1,226,000): NSF ACI-1339804. Collaboration with IBM (Dr. Glenn Martyna) and UIUC (Prof. Sanjay Kalé) to enhance the OpenAtom highly scalable parallel software. Funds two postdocs in Ismail-Beigi group.

- Control and Design of Two Dimensional Silica Structures, (PI Eric Altman, co-PIs Udo Schwarz and Sohrab Ismail-Beigi, 9/1/2015-8/31-2018, \$475,000): NSF DMR-1506800. Funds one half graduate student in Ismail-Beigi group.
- Dynamically configurable memory technology based on ferroelectric-gated field effect transistors, (PI Tso-Ping Ma, co-PI Sohrab Ismail-Beigi), 9/1/2016-8/31/2019, \$345,000): NSF/ENG/ECCS-BSF 1609162. Funds one graduate student in Ismail-Beigi group.
- Subaward from the UCLA “Functional Accelerated Nano-Material Engineering (FAME)” research center award (MARCO Contract No. 2013-MA-2382 from the Microelectronics Advanced Research Corporation), 11/01/2015-10/31/2016, \$160,000 per year (anticipated to be for two years until 10/31/2017). Funds one postdoc in Ismail-Beigi’s group.

#### Previous Funding

- First Principles Investigations of Boron Nanostructures (PI Sohrab Ismail-Beigi, 9/2011-08/2014, \$300,000, no-cost extension until 2016): NSF DMR-1104974. Supported one graduate student in Ismail-Beigi group.
- Enhancement of NO<sub>x</sub> Decomposition Through Ferroelectric Supports (PI Eric Altman, 07/2011-12/2014, \$149,709/year): Toyota Motor Engineering and Manufacturing, North America, Inc. Supported one graduate student in Ismail-Beigi group.
- Atomic Engineering of Superconductors by Design (PI Charles Ahn, 6/2010-07/2013, \$449,885/year): DOD DARPA W911NF-10-1-0206. Supported one graduate student or postdoc in Ismail-Beigi group.
- Founding co-PI on NSF DMR-0520495 MRSEC/Materials Research Science and Engineering Center for Research on Interface Structures and Phenomena (PI John Tully, 10/2005-09/2011, \$6,390,000 total). Supported two graduate students in Ismail-Beigi group and one joint postdoctoral fellow in Ismail-Beigi and Tully groups.
- NSF DMR-0808665: First Principles Investigations of Boron Nanostructures (PI Sohrab Ismail-Beigi, 9/2008-08/2011, \$240,000). Supported one graduate student in Ismail-Beigi group.
- Acquisition of a High Performance Computational Cluster for Yale University (PI Steven Girvin, 7/2008-6/2012, \$500,000): NSF MRI CNS-0821132. Allowed for the acquisition of the Bulldog L FAS HPC computer cluster.
- SOLAR: Novel Nanomaterials, Assembly and Mathematical Analysis for Ultra-High Efficiency Photovoltaic Systems: A New Paradigm in Solar Cells (PI Lisa Pfefferele, 8/2009-7/2012, \$1,143,530): NSF DMR 0934520. Supported one postdoctoral fellow in Ismail-Beigi group.

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## PUBLICATIONS, THESES, AND PATENTS

(electronic version with hyperlinks at <http://volga.eng.yale.edu/sohrab/cv/cv.html#publications>)  
(PDF version has hyperlinks: click on journal names)

1. A. Antonelli, S. Ismail-Beigi, E. Kaxiras, and K. C. Pandey, “Free energy of concerted-exchange mechanism for self-diffusion in silicon”, *Physical Review B* **53**, 1310 (1996).
2. S. Ismail-Beigi and T. A. Arias, “Edge-driven transition in surface structure of nanoscale silicon”, *Physical Review B* **57**, 11923 (1998).
3. G. Csányi, S. Ismail-Beigi, and T. A. Arias, “Paramagnetic Structure of the Soliton of the 30° Partial Dislocation in Silicon”, *Physical Review Letters* **80**, 3984 (1998).

4. S. Ismail-Beigi and T. A. Arias, "Locality of the Density Matrix in Metals, Semiconductors and Insulators", *Physical Review Letters* **82**, 2127 (1999).
5. S. Ismail-Beigi and T. A. Arias, "Ab Initio Study of Screw Dislocations in Mo and Ta: A new picture of plasticity in bcc transition metals", *Physical Review Letters* **84**, 1499 (2000).
6. S. Ismail-Beigi and T. A. Arias, "New Algebraic Formulation of Density Functional Calculation", *Computer Physics Communications* **128**, 1-45 (June 2000).
  - Invited paper for special issue of *Computer Physics Communications* on "Parallel Computing in Chemical Physics".
7. S. Ismail-Beigi, P. Marrone, M. Reagan, T. A. Arias, and J. Tester, "Ab Initio approach to continuum calculations of solvation energies in water", (part of Ph.D. thesis, 2000). <http://arxiv.org/abs/cond-mat/0007514>
8. G. Csányi, T. D. Engeness, S. Ismail-Beigi, and T. A. Arias, "New Physics of the 30° Partial Dislocation in Silicon", *Journal of Physics: Condensed Matter* **12**, 10029 (2000).
9. S. Ismail-Beigi, E. K. Chang, S. G. Louie, "Coupling of Nonlocal Potentials to Electromagnetic Fields", *Physical Review Letters* **87**, 087402 (2001).
10. D. E. Segall, S. Ismail-Beigi, and T. A. Arias, "Elasticity of nanometer-sized objects", *Physical Review B* **65**, 214109 (2002).
11. W. Luo, S. Ismail-Beigi, M. L. Cohen, and S. G. Louie, "Quasiparticle band structure of ZnS and ZnSe", *Physical Reviews B* **66**, 195215 (2002).
12. D. S. Segall, S. Ismail-Beigi, A. Strachan, W. A. Goddard III, and T. A. Arias, "Ab Initio and Finite Temperature Molecular Dynamics Studies of Lattice Resistance in Tantalum", *Physical Reviews B* **68**, 014104 (2003).
13. S. Ismail-Beigi and S. G. Louie, "Excited-state Forces within the Ab Initio Bethe-Salpeter Formalism", *Physical Reviews Letters* **90**, 076401 (2003).
14. C. D. Spataru, S. Ismail-Beigi, L. X. Benedict, and S. G. Louie, "Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes", *Physical Reviews Letters* **92**, 077402 (2004).
15. C. D. Spataru, S. Ismail-Beigi, L. X. Benedict, and S. G. Louie, "Quasiparticle energies, excitonic effects, and optical absorption of small-diameter single-walled carbon nanotubes", invited contribution to *Applied Physics A* **78**, 1129 (2004).
16. M. L. Tiago, S. Ismail-Beigi, and S. G. Louie, "Effect of semicore orbitals on the electronic band gaps of Si, Ge, and GaAs within the GW approximation", *Physical Review B* **69**, 125212 (2004).
17. M. L. Tiago, S. Ismail-Beigi, and S. G. Louie, "Photoisomerization of azobenzene from first-principles constrained density-functional calculations", *Journal of Chemical Physics* **122**, 094311 (2005).
18. S. Ismail-Beigi and S. G. Louie, "Self-trapped Excitons in Silicon Dioxide: Mechanisms and Properties", *Physical Review Letters* **95**, 156401 (2005).
19. C. D. Spataru, S. Ismail-Beigi, R. B. Capaz, and S. G. Louie, "Theory and *Ab Initio* Calculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes", *Physical Review Letters* **95**, 247402 (2005).
20. E. B. Barros, R. B. Capaz, A. Jorio, G. G. Samsonidze, A. G. Souza Filho, S. Ismail-Beigi, C. D. Spataru, S. G. Louie, G. Dresselhaus, and M. S. Dresselhaus, "Selection rules for one- and two-photon absorption by excitons in carbon nanotubes", *Physical Review B* **73**, 241406 (2006).

21. R. B. Capaz, C. D. Spataru, S. Ismail-Beigi, and S. G. Louie, "Diameter and chirality dependence of exciton properties in carbon nanotubes", *Physical Review B* **74**, 121401 (2006).
22. S. Ismail-Beigi, "Truncation of periodic image interactions for confined systems", *Physical Review B* **73**, 233103 (2006).
23. H. Tang and S. Ismail-Beigi, "Novel Precursors for Boron Nanotubes: The Competition of Two-Center and Three-Center Bonding in Boron Sheets", *Physical Review Letters* **99**, 115501 (2007).
  - Selected as an Editor's Suggestion in *Physical Review Letters*.
  - Highlighted in "Search and Discovery" of *Physics Today* **60** (November/issue 11), 20 (2007) (PDF)
  - Featured interview in PhysOrg.com (Sept. 27, 2007).
24. R. B. Capaz, C. D. Spataru, S. Ismail-Beigi, and S. G. Louie, "Excitons in carbon nanotubes: Diameter and chirality trends", *Physica Status Solidi (b)* **11**, 4016 (2007).
25. A. Sitt, L. Kronik, S. Ismail-Beigi, and J. R. Chelikowsky, "Excited-state forces within time-dependent density-functional theory: A frequency-domain approach" *Physical Review A* **76**, 054501 (2007).
26. S. Ismail-Beigi, "Electronic excitations in single-walled gallium nitride nanotubes from first principles: dark excitons and unconventional diameter dependences", *Physical Review B* **77**, 035306 (2008).
27. J. W. Reiner, K. F. Garrity, F. J. Walker, S. Ismail-Beigi, and C. H. Ahn, "Role of Strontium in Oxide Epitaxy on Silicon (001)", *Physical Review Letters* **101**, 105503 (2008).
28. Y. Segal, J. W. Reiner, A. M. Kolpak, Z. Zhang, S. Ismail-Beigi, C. H. Ahn, and F. J. Walker, "Atomic Structure of the Epitaxial BaO/Si(001) Interface", *Physical Review Letters* **102**, 116101 (2009).
29. H. Chen, A. M. Kolpak, and S. Ismail-Beigi, "Fundamental asymmetry in interfacial electronic reconstruction between insulating oxides: An *ab initio* study", *Physical Review B* **79**, 161402(R) (2009).
30. K. Garrity and S. Ismail-Beigi, "Phase diagram of Sr on Si(001): A first-principles study", *Physical Review B* **80**, 085306 (2009).
  - Selected as an Editor's Suggestion in *Physical Review B*.
31. H. Tang and S. Ismail-Beigi, "Self-doping in boron sheets from first principles: A route to structural design of metal boride nanostructures", *Physical Review B* **80**, 134113 (2009).
32. J. W. Reiner, Y. Segal, K. F. Garrity, H. Hong, S. Ismail-Beigi, C. H. Ahn and F. J. Walker, "Diffraction studies of submonolayer Sr structures on the Si (001) surface", *Journal of Vacuum Science and Technology* **27**, 2015 (2009).
33. K. F. Garrity, M.-R. Padmore, Y. Segal, J. W. Reiner, F. J. Walker, C. H. Ahn and S. Ismail-Beigi, "Phase transition of Sr on Si (001): First principles prediction and experiment", *Surface Science* **604**, 857 (2010).
34. A. Lubow, S. Ismail-Beigi, and T. P. Ma, "Comparison of Drive Currents in Metal-Oxide-Semiconductor Field-Effect Transistors Made of Si, Ge, GaAs, InGaAs and InAs Channels", *Applied Physics Letters* **96**, 122105 (2010).
  - Featured in *Semiconductor Today* April 1, 2010 issue.
35. S. Ismail-Beigi, "Correlation energy functional within the GW-RPA: Exact forms, approximate forms, and challenges", *Physical Review B* **81**, 195126 (2010).

36. J. H. Ngai, Y. Segal, D. Su, Y. Zhu, F. J. Walker, S. Ismail-Beigi, K. Le Hur, and C. H. Ahn, “Electric field tuned crossover from classical to weakly localized quantum transport in electron doped SrTiO<sub>3</sub>”, *Physical Review B Rapid Communications* **81**, 241307(R) (2010).

★ Entire Special Issue of *Advanced Materials* is devoted to Yale’s CRISP NSF-MRSEC center (*Advanced Materials* Volume 22 Issue 26-27, July 2010). Relevant articles are the following three.

- 37 H. Chen, A. M. Kolpak, and S. Ismail-Beigi, “Electronic and Magnetic Properties of SrTiO<sub>3</sub>/LaAlO<sub>3</sub> Interfaces from First Principles”, *Advanced Materials* **22** 2881-2899 (2010).
- 38 J. W. Reiner, A. M. Kolpak, Y. Segal, K. F. Garrity, S. Ismail-Beigi, C. H. Ahn, and F. J. Walker, “Crystalline Oxides on Silicon”, *Advanced Materials* **22** 2919-2938 (2010).
- 39 K. Garrity, A. M. Kolpak, S. Ismail-Beigi, and E. I. Altman, “Chemistry of Ferroelectric Surfaces”, *Advanced Materials* **22**, 2969-2973 (2010).
40. H. Chen, A. M. Kolpak, S. Ismail-Beigi, “First-principles study of electronic reconstructions of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterointerfaces and their variants”, *Physical Review B* **82**, 085430 (2010).
41. H. Tang and S. Ismail-Beigi, “First-principles study of boron sheets and nanotubes”, *Physical Review B* **82**, 115412 (2010).
42. A. M. Kolpak, F. J. Walker, J. W. Reiner, Y. Segal, D. Su, M. S. Sawicki, C. C. Broadbridge, Z. Zhang, Y. Zhu, C. H. Ahn, and S. Ismail-Beigi, “Interface-Induced Polarization and Inhibition of Ferroelectricity in Epitaxial SrTiO<sub>3</sub>/Si”, *Physical Review Letters* **105**, 217601 (2010).
- Chosen for a synopsis highlight in *Physics*
  - Selected as an Editor’s Suggestion in *Physical Review Letters*.
  - Featured on November 18 2010 Materials Research Society’s *Materials News*
43. A. M. Kolpak and S. Ismail-Beigi, “Thermodynamic stability and growth kinetics of epitaxial SrTiO<sub>3</sub> on silicon”, *Physical Review B* **83**, 165318 (2011).
- Selected as an Editor’s Suggestion in *Physical Review B*.
44. Y. Segal, K. F. Garrity, C. A. F. Vaz, J. D. Hoffman, F. J. Walker, S. Ismail-Beigi, and C. H. Ahn, “Dynamical Evanescent Phonon Coupling Across the La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>/SrTiO<sub>3</sub> Interface”, *Physical Review Letters* **107**, 105501 (2011).
45. S. Zhang, C. I. Pelligra, G. Keskar, J. Jiang, P. W. Majewski, A. D. Taylor, S. Ismail-Beigi, L. D. Pfefferle and C. O. Osuji, “Directed Self-Assembly of Hybrid Oxide/Polymer Core-Shell Nanowires with Transport Optimized Morphology for Photovoltaics”, *Advanced Materials* online (2011) and in print **24**, 82 (2012)
46. B. Lukanov, K. Garrity, S. Ismail-Beigi and E. I. Altman, “Deciphering the atomic structure of a complex Sr/Ge(100) phase via scanning tunneling microscopy and first-principles calculations”, *Physical Review B* **85**, 195316 (2012).
47. A. M. Kolpak and S. Ismail-Beigi, “Interface structure and film polarization in epitaxial SrTiO<sub>3</sub>/Si(001)”, *Physical Review B* **85**, 195318 (2012).
48. Kevin F. Garrity, Alexie M. Kolpak and Sohrab Ismail-Beigi, “Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights”, invited review article for *Journal of Materials Science* **47** 7417 (2012). DOI: 10.1007/s10853-012-6425-z.
49. H. Chen and S. Ismail-Beigi, “Ferroelectric control of magnetization in La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> manganites: A first-principles study”, *Physical Review B* **86**, 024433 (2012).

50. Hanghui Chen, Divine P. Kumah, Ankit S. Disa, Frederick J. Walker, Charles H. Ahn and Sohrab Ismail-Beigi, "Modifying the Electronic Orbitals of Nickelate Heterostructures via Structural Distortions", *Physical Review Letters* **110**, 186402 (2013).
51. Kevin Garrity, Arvin Kakekhani, Alexie Kolpak and Sohrab Ismail-Beigi, "Ferroelectric surface chemistry: First-principles study of the  $\text{PbTiO}_3$  surface", *Physical Review B* **88**, 045401 (2013).
52. Seyla Azoz, Jie Jiang, Gayatri Keskar, Charles McEnally, Alp Alkas, Fang Ren, Nebojsa Marinkovic, Gary L. Haller, Sohrab Ismail-Beigi and Lisa D. Pfefferle, "Mechanism for strong binding of CdSe quantum dots to multiwall carbon nanotubes for solar energy harvesting", *Nanoscale* **5**, 6893 (2013).
53. Divine P. Kumah, Ankit S. Disa, Joseph H. Ngai, Hanghui Chen, Andrei Malashevich, James W. Reiner, Sohrab Ismail-Beigi, Frederick J. Walker, Charles H. Ahn, "Tuning the Structure of Nickelates to Achieve Two-Dimensional Electron Conduction", *Advanced Materials* **26**, 1935 (2014).
54. Xiaokai Li, Louise M. Guard, Jie Jiang, Kelsey Sakimoto, Jing-Shun Huang, Jianguo Wu, Jinyang Li, Lianqing Yu, Ravi Pokhrel, Gary W. Brudvig, Sohrab Ismail-Beigi, Nilay Hazari, and André D. Taylor, "Controlled Doping of Carbon Nanotubes with Metallocenes for Application in Hybrid Carbon Nanotube/Si Solar Cells", *Nano Letters* **14**, 3388 (2014).
55. Boris R. Lukanov, Kevin F. Garrity, Sohrab Ismail-Beigi, and Eric I. Altman, "Formation and atomic structure of ordered Sr-induced nanostrips on  $\text{Ge}(100)$ ", *Physical Review B* **89**, 155319 (2014).
56. Hanghui Chen, Qiao Qiao, Matthew S. J. Marshall, Alexandru B. Georgescu, Ahmet Gulec, Patrick Phillips, Robert F. Klie, Frederick J. Walker, Charles H. Ahn and Sohrab Ismail-Beigi, "Reversible Modulation of Orbital Occupations via an Interface-Induced Polar State in Metallic Manganites", *Nano Letters* **14**, 4965 (2014).
57. D. P. Kumah, A. Malashevich, A. S. Disa, D. A. Arena, F. J. Walker, S. Ismail-Beigi, and C. H. Ahn, "Effect of Surface Termination on the Electronic Properties of  $\text{LaNiO}_3$  Films", *Physical Review Applied* **2** (2014).
58. A. Malashevich, E. I. Altman, and S. Ismail-Beigi, "Imaging the buried  $\text{MgO}/\text{Ag}$  interface: Formation mechanism of the STM contrast", *Physical Review B* **90** (2014).
59. Matthew S. J. Marshall, Andrei Malashevich, Ankit S. Disa, Myung-Geun Han, Hanghui Chen, Yimei Zhu, Sohrab Ismail-Beigi, Frederick J. Walker, and Charles H. Ahn, "Conduction at a Ferroelectric Interface", *Physical Review Applied* **2**, 051001 (2014).
60. A. S. Disa, D. P. Kumah, A. Malashevich, H. Chen, D. A. Arena, E. D. Specht, S. Ismail-Beigi, F. J. Walker, and C. H. Ahn, "Orbital Engineering in Symmetry-Breaking Polar Heterostructures", *Physical Review Letters* **114**, 026801 (2015).
  - Selected as an Editor's Suggestion in *Physical Review Letters*.
  - Highlighted as an *APS Physics Viewpoint*.
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61. C. A. F. Vaz, F. J. Walker, C. H. Ahn and S. Ismail-Beigi, "Intrinsic interfacial phenomena in manganite heterostructures", *Journal of Physics: Condensed Matter* **27**, 123001 (2015). DOI 10.1088/0953-8984/27/12/123001.
62. K. Zou, Sohrab Ismail-Beigi, Kim Kisslinger, Xuan Shen, Dong Su, F. J. Walker and C. H. Ahn, " $\text{LaTiO}_3/\text{KTaO}_3$  interfaces: A new two-dimensional electron gas system", *APL Materials* **3**, 036104 (2015). DOI 10.1063/1.4914310.
63. Thomas A. Mellan, Furio Cora, Ricardo Grau-Crespo and Sohrab Ismail-Beigi, "Importance of anisotropic Coulomb interaction in  $\text{LaMnO}_3$ ", *Physical Review B* **92**, 085151 (2015). DOI 10.1103/PhysRevB.92.085151 Preprint from on arxiv at [arxiv.org/abs/1503.08871](https://arxiv.org/abs/1503.08871).

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65. Sohrab Ismail-Beigi, Frederick J. Walker, Sang-Wook Cheong, Karin M. Rabe and Charles H. Ahn, "Alkaline earth stannates: The next silicon?", *APL Materials* **3**, 062510 (2015). DOI 10.1063/1.4921338. This is open-access and available to read on the website.
66. Arvin Kakekhani and Sohrab Ismail-Beigi, "Ferroelectric-Based Catalysis: Switchable Surface Chemistry", *ACS Catalysis* **5**, 4537-4545 (2015). DOI 10.1021/acscatal.5b00507. The PDF available as per ACS AuthorChoice open-access.
67. Andrei Malashevich and Sohrab Ismail-Beigi, "First-principles study of oxygen-deficient LaNiO<sub>3</sub> structures", *Physical Review B* **92**, 144102 (2015). DOI 10.1103/PhysRevB.92.144102
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73. Ke Zou, Subhasish Mandal, Stephen D. Albright, Rui Peng, Yulia Pu, Divine P. Kumah, Claudia Lau, Georg Simon, Omur E. Dagdeviren, Xi He, Ivan Bozovic, Udo D. Schwarz, Eric I. Altman, Dlonglai Feng, Frederick J. Walker, Sohrab Ismail-Beigi, and Charles H. Ahn, "Role of double TiO<sub>2</sub> layers at the interface of FeSe/SrTiO<sub>3</sub> superconductors", *Physical Review B* **93**, 180506 (2016). DOI 10.1103/PhysRevB.93.180506
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80. Patrick J. Phillips, Xue Rui, Alexandru B. Georgescu, Ankit S. Disa, Paolo Longo, Eiji Okunishi, Fred Walker, Charles H. Ahn, Sohrab Ismail-Beigi, and Robert F. Klie”, “Experimental verification of orbital engineering at the atomic scale: charge transfer and symmetry breaking in nickelate heterostructures”, *Physical Review B*, vol. 95, 205131 (2017). DOI 10.1103/PhysRevB.95.205131. Arxiv version <https://arxiv.org/abs/1612.05610>
81. Sohrab Ismail-Beigi, “Justifying quasiparticle self-consistent schemes via gradient optimization in Baym-Kadanoff theory”, *Journal of Physics: Condensed Matter* vol. 29, 385501 (2017). DOI 10.1088/1361-648X/aa7803 Arxiv version <https://arxiv.org/abs/1406.0772>
82. Ankit S. Disa, Alexandru B. Georgescu, James L. Hart, Divine P. Kumah, Padraic Shafer, Elke Arenholz, Daio A. Arena, Sohrab Ismail-Beigi, Mitra L. Taheri, Frederick J Walker, and Charles H. Ahn, “Control of hidden ground-state order in NdNiO<sub>3</sub> superlattices”, *Physical Review Materials* vol. 1, 024410 (2017). DOI 10.1103/PhysRevMaterials.1.024410
  - Selected as an Editor’s Suggestion in *Physical Review Materials*.
83. Mehmet Dogan and Sohrab Ismail-Beigi, “*Ab initio* study of the BaTiO<sub>3</sub>/Ge interface”, *Physical Review B* vol. 96, 075301 (2017). DOI 10.1103/PhysRevB.96.075301
  - Selected as an Editor’s Suggestion in *Physical Review B*.
84. A. Georgescu and S. Ismail-Beigi, “Symmetry Breaking in Slave-Particle Methods for the Hubbard Model”, (2017) arXiv:1702.03381
85. Minjung Kim, Glenn J Martyna, Sohrab Ismail-Beigi, “Imaginary time, shredded propagator method for large-scale GW calculations”, (2017) <https://arxiv.org/abs/1707.06752>.

### Conference proceedings and book chapters

- S. Ismail-Beigi, “First principles calculation of optical and electronic properties with inclusion of exciton effects”, *Physica Status Solidi (c)* **3**, 3365 (2006).
- Chapter 6 on electronic excitations in carbon nanotubes as part of the second edition by Springer of “Carbon Nanotubes: Advanced Topics in the Synthesis, Structure, Properties and Applications” with co-authors C. D. Spataru, R. B. Capaz, and S. G. Louie. Edited by Ado Jorio, Gene Dresselhaus and Mildred S. Dresselhaus (2008).
- Chapter 3 on “Two-Dimensional Boron Sheets” in the book “Handbook of Boron Nanostructures” edited by Sumit Saxena. Pan Stanford publishing (2016).

### Theses

- Sohrab Ismail-Beigi, “New Perspectives on *Ab Initio* Calculation and Physical Insights Through Linkage to Continuum Theories”, Ph.D. thesis in Physics, Massachusetts Institute of Technology, June 2000. PDF
- Kevin F. Garrity, “*Ab Initio* Studies of Surfaces and Interfaces”, Ph.D. thesis in Physics, Yale University, May 2011. PDF
- Hui Tang, “First Principles Investigations of Boron Nanostructures”, Ph.D. thesis in Applied Physics, Yale University, May 2011. PDF



- Hanghui Chen, “A First Principles Study on Oxide Interfaces”, Ph.D. thesis in Physics, Yale University, May 2012. PDF
- Arvin Kakekhani, “Using Ferroelectrics to Tackle Fundamental Challenges in Catalysis”, Ph.D. thesis in Physics, Yale University, May 2016. PDF

#### Patents

- A. M. Kolpak, F. J. Walker, J. W. Reiner, C. H. Ahn, and S. Ismail-Beigi, “Ferroelectric Devices including a Layer having Two or More Stable Configurations”, US Patent number 9536975, Application number 14/745,457 (2017).

## 4. HONORS AND INVITED PRESENTATIONS

- Winner of a Certificate of Distinction in Teaching Award (*Spring 1992*).
- Elected to Phi Beta Kappa as a Junior (*Spring 1992*).
- Graduated *summa cum laude* from Harvard University (highest academic ranking) (*June 1993*).
- Winner of the Hoopes Prize for excellence in undergraduate research in Physics. Thesis title: “Development of a New Interatomic Potential for silicon”; under the direction of Prof. Efthimios Kaxiras, Dept. of Physics (*June 1993*).
- Funding for Studies in Lyon provided by a Rotary International Ambassadorial Scholarship (*September 1993-June 1994*).
- IBM Faculty Award (*2006*).

Invited talks and/or keynote presentations:

- The Workshop on Recent Developments in Electronic Structure Methods, Atlanta, GA (*May 2000*).
- The Workshop on Recent Developments in Electronic Structure Methods, Princeton, NJ (*June 2001*).
- The 11th International Workshop on Computational Physics and Materials Science, Trieste, Italy (*January 2003*).
- Theory and Modeling of Electronic Excitations in Nanoscience Conference, Acquafredda di Maratea, Italy (*September 2004*).
- Yale Physics Club Colloquium (*January 21, 2005*).
- Workshop on Recent Developments in Electronic Structure Methods, Cornell, NY (*June 2005*).
- Department of Materials and Interfaces seminar speaker, Weizmann Institute, Israel (*January 2006*).
- The American Ceramics Society GOMD Spring meeting, Greenville, SC (*May 2006*).
- Excitonic Processes in Condensed Matter Conference, Winston-Salem, NC (*June 2006*).
- Computational Methods for Nanoscale Systems, Hong Kong (*December 2006*).
- Laboratory for Surface Modification Seminar, Rutgers University, NJ (*February 2007*).
- Laboratory for Research on the Structure of Matter Seminar, University of Pennsylvania, PA (*March 2007*).

- Computational Materials Seminar, Cornell University, NY (*April 2007*).
- Condensed Matter Seminar, Case Western Reserve University, OH (*January 2008*).
- Physics Colloquium, SUNY Buffalo, NY (*March 2008*).
- Physical Science Seminar, IBM Yorktown, NY (*May 2008*).
- Time-Dependent Density-Functional Theory: Prospects and Applications, Benasque, Spain (*September 2008*).
- 15th International Workshop on Oxide Electronics, Estes Park, Colorado (*September 2008*).
- Molecular Foundry & NCEM Users' Workshop 2008, Berkeley (*November 2008*).
- BECAT-IBM Workshop on High Performance Computational Science and Engineering, U. Conn. Storrs (*December 2008*).
- The 2nd International Workshop: Nanoxide (oxide interfaces), Valbella Grisons, Switzerland (*April 2009*).
- 16th International Workshop on Oxide Electronics, Tarragona, Spain (*October 2009*).
- Physical Chemistry Seminar, University of Pennsylvania, PA (*January 20, 2011*).
- CECAM/Psi-k Workshop on Challenges and solutions in GW calculations for complex systems, Lausanne, Switzerland (*June 2011*).
- Computational Surface Science 2011 Workshop, Santa Barbara (*August 2011*).
- Applied Physics Seminar, Harvard University, MA (*October 21, 2011*).
- Materials Science and Engineering Colloquium, Columbia University, NY (*November 4, 2011*).
- Condensed Matter/Materials and Biological Physics Seminar, Washington University in St. Louis, MO (*December 12, 2011*).
- March APS Meeting, Boston, MA (*March, 2012*).
- The 24th Annual Workshop on Recent Developments in Electronic Structure Theory, Wake Forest University, Winston-Salem, NC (*June 2012*).
- CECAM/Psi-k Workshop on What about U? - Corrective approaches to DFT for strongly-correlated systems, Lausanne, Switzerland (*June 2012*).
- Santorini II in Mallorca: Workshop on the Physics of Complex Oxides, Mallorca, Spain (*October 2012*).
- AVS meeting (59<sup>th</sup> in Tampa Florida), session on Structure Property Relationships in Epitaxial Oxide Interfaces, Tampa, FL (*November 2012*). (Talk canceled due to Hurricane Sandy)
- 290K Condensed Matter Seminar, Department of Physics, University of California at Berkeley, Berkeley, CA (*February 2013*).
- Physics Colloquium, University of Illinois at Chicago (UIC) (*March 2013*).
- German Physical Society (DPG) Spring meeting 2013, Regensburg, Germany (*March 2013*).
- Telluride Workshop 2013 on Physics of Emergent Correlated Materials, Telluride Science Center, Telluride, CO (*June 2013*).
- Hayashi Conference: Next decades of Surface Science, Shonan Village Center, Hayama, Japan (*July 2013*).

- Materials for a Sustainable Energy Future: Fuels from Sunlight (Workshop II), Institute for Pure and Applied Mathematics, University of California at Los Angeles, CA (*October 2013*).
- Physics at the Falls: Structural and Electronic Instabilities in Oxide Nanostructures, SUNY Buffalo, Buffalo, NY (*May 2014*).
- American Chemical Society Fall meeting 2014, invited talk, San Francisco, CA (*August 2014*).
- Physics Colloquium, Temple University, Philadelphia, PA (*September 2014*).
- March APS Meeting, San Antonio, TX (*March, 2015*).
- The 8<sup>th</sup> Workshop for Emergent Materials Research, POSTECH University, Pohang, South Korea (*July, 2015*).
- Materials Science and Engineering Colloquium, University of Illinois at Urbana-Champaign (UIUC), Urbana-Champaign, IL (*November 2015*).
- NSF-MolSSI Sponsored Workshop on Materials Software, Berkeley, CA (*February, 2017*).
- March APS Meeting, New Orleans, LA (*March, 2017*).

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## 5. INTERNATIONAL COLLABORATORS

Prof. H.-C. Hsueh (Department of Physics, Tamsui University, Taiwan): began a collaboration based on an invited ten day visit to Taiwan (*Spring 2004*).

Prof. Leer Kronik (Department of Materials and Interfaces, Weizmann Institute): began a collaboration based on an invited two week visit to Israel (*January 2006*).

Dr. Yoshifumi Noguchi (Department Physics, Tokyo University): visited Ismail-Beigi group in fall of 2011 as a visiting scholar and began collaboration on photovoltaics project.

Mr. Thomas Mellan and Prof. Ricardo Grau-Crespo (Department of Chemistry, Univeristy College London): Mr. Mellan, a graduate student supervised by Prof. Grau-Crespo, visited CRISP and Yale March-May 2013 to begin a research collaboration on the physics of manganite thin films and heterostructures.

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## 6. RESEARCH SUPERVISION

	Name	Department	Project	Semester/Years
High school teachers	Kenneth Spinka	New Haven Public Schools	course development	2009 Summer
	Charmel Moore	New Haven Public Schools	TEM analysis	2016 Summer
Undergrad	Caitlin Lonegan	Applied Physics	senior project	2004 Fall
	Caitlin Lonegan	Applied Physics	senior project	2005 Spring
	Eli Luberoff	—	Persp. in Sci.*	2005 Summer
	Yejin Huh	Physics	summer project	2005 Summer
	Yejin Huh	Physics	senior thesis	2005 Fall
	Yejin Huh	Physics	senior thesis	2006 Spring
	Madeleine Udell	—	Persp. in Sci.*	2006 Summer
	Stephen Fedele	Applied Physics	senior project	2006 Fall
	Stephen Fedele	Applied Physics	senior project	2007 Spring
	Torrey-Levin Russel	SCSU Physics	REU	2009 Summer
	Torrey-Levin Russel	SCSU Physics	research class	2009 Fall
	Torrey-Levin Russel	SCSU Physics	research class	2010 Spring
	Diana Qiu	Physics	senior thesis	2010 Fall
	Sheide Chammas	Applied Physics	senior project	2010 Fall
	Sheide Chammas	Applied Physics	senior project	2011 Spring
	Ismail Elbaggari	Applied Physics	summer project	2011 Summer
	Ismail Elbaggari	Applied Physics	senior project	2011 Fall
	Ismail Elbaggari	Applied Physics	senior project	2012 Spring
	Ismail Elbaggari	Applied Physics	summer project	2012 Summer
	Alexis Morris	Truman State U.	REU	2013 Summer
	Michael Onyszczyk	Iowa State U.	REU	2015 Summer
	Dylan Young	Physics	summer project	2016 Summer
Dylan Young	Physics	research course	2016 Fall	
Graduate	Hui Tang	Applied Physics	Ph.D. thesis	2006-2011
	Kevin Garrity	Physics	Ph.D. thesis	2006-2011
	Hanghui Chen	Physics	Ph.D. thesis	2007-2012
	Arvin Kakekhani	Physics	Ph.D. thesis	2011-2016
	Mehmet Dogan	Physics	Ph.D. thesis	2012-2017
	Alexandru Georgescu	Physics	Ph.D. thesis	2012-2017
	Xin Liang	Applied Physics	Ph.D. thesis	2012-present
	Thomas Mellan	visitor	research	March-May 2013
	Stephen Eltinge	Physics	Ph.D. thesis	2015-present
Postdoctoral	Dr. Alexie Kolpak	Applied Physics	CRISP (NSF)	2007-2010
	Dr. Jie Jiang	Applied Physics	SOLAR (NSF)	2010-2013
	Dr. Andrei Malashevich	Applied Physics	CRISP (NSF) & DARPA	2012-2015
	Dr. Minjung Kim	Applied Physics	SI2-SSI (NSF)	2014-present
	Dr. Subhasish Mandal	Applied Physics	SI2-SSI (NSF)	2014-present

\* Perspectives in Science

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## 7. TEACHING

Course number	Abbreviated title	semester
ENAS 856a	Theory of Solids I	2003 Fall
ENAS 856a	Theory of Solids I	2004 Fall
PHYS 165La	General Physics Lab	2004 Fall
ENAS 194a	Differential Equations with Applications	2005 Fall
PHYS 166a	General Physics Lab	2006 Spring
ENAS 194a	Differential Equations with Applications	2006 Fall
ENAS 993	Theory of Solids I Seminar	2006 Fall
SCIE 198	Perspectives in Science	2007 Fall
APHY 439	Basic Quantum Mechanics	2008 Fall
PHYS 181	Advanced General Physics	2009 Spring
ENAS 194a	Differential Equations with Applications	2010 Fall
PHYS 181	University Physics	2011 Spring
PHYS 181	University Physics	2012 Spring
APHY 439	Basic Quantum Mechanics	2012 Fall
APHY 650	Theory of Solids I Reading	2012 Fall
APHY/ENAS 151	Multivariable Calculus for Engineers	2013 Spring
APHY 993	Topics in DFT and First Principle Methods	2013 Fall
APHY/ENAS 151	Multivariable Calculus for Engineers	2014 Spring
APHY/ENAS 151	Multivariable Calculus for Engineers	2014 Fall
APHY/PHYS 650	Theory of Solids I	2015 Fall
APHY/PHY 449/549	Solid-State Physics II	2016 Spring
APHY 439	Basic Quantum Mechanics	2016 Fall

## 8. SERVICE TO YALE

**FAS and ITS High Performance Computing (HPC) committees:** are composed of faculty, administrators, and ITS staff and are responsible for setting the direction of HPC computation in FAS. They plan major hardware and software acquisitions, set and enforce policies regarding access and use of HPC facilities, resolve user problems, prepare plans for modifications and improvements of the facilities, and act as the highest authority in FAS regarding HPC planning, issues, and concerns. From 2007-2013, there were two committees: a larger one chaired by the Deputy Provost Prof. Steven Girvin which met relatively infrequently to vote on major issues or discuss long-range plans. A second HPC subcommittee was co-chaired by Profs. Paolo Coppi and Sohrab Ismail-Beigi and met on average once or twice a month and prepared drafts of long-term plans, answered user concerns and questions, got regular updates from ITS, drafted modifications of current policies to ensure fair HPC usage by all users, etc. Since the summer of 2013, the committees were reorganized and Ismail-Beigi became a member of the formed Planning Committee. Since 2015, Yale formed the Yale Center for Research Computing to provide permanence and continuity to HPC efforts at Yale, and Ismail-Beigi is a member of the Steering Committee.

Committee	Function	Semester
HPC committee	member	2007-2013
HPC subcommittee	co-chair	2007-2013
HPC committee	selection committee member and interviewer for two HPC technical positions	2008 Spring
HPC Operations and Planning Committee	member	2013-2014
Yale Center for Research Computing Steering Committee	member	2015-present
Yale Committee on Procedures for Faculty Misconduct	member	2016-present

### Seminar series organizer

Organization	Seminar series	Semester
Applied Physics	Solid State and Optics Seminar	2006-2008, Spring & Fall
Applied Physics	Monday Evening Graduate Student Seminar	2006-2008, Spring & Fall
CRISP	CRISP internal and external seminars	2005-2011
CRISP	CRISP IRG1 internal and external seminars	2011-present

**Departmental committees (admissions, faculty searches, qualifying exams)**

Department	Function	Semester
Applied Physics	graduate admissions committee member	2004 Spring
Physics	Qualifying Exam committee	2005 Fall
Applied Physics	graduate admissions committee member	2005 Spring
Applied Physics	graduate admissions committee member	2006 Spring
Applied Physics	Junior Optics Search Committee member	2007 Spring
Physics	graduate admissions committee member	2008 Spring
Applied Physics	graduate admissions phone interviews	2008 Spring
Applied Physics	graduate admissions phone interviews	2009 Spring
Applied Physics	graduate admissions phone interviews	2011 Spring
Physics	graduate admissions committee member	2011 Spring
Physics	Qualifying Exam committee	2011 Fall
Mech. Eng. & Mat. Sci	Faculty Search Committee member	2011 Fall-present
Applied Physics	graduate admissions committee member	2013 spring
Physics	Qualifying Exam committee	2013 Fall
Applied Physics	graduate admissions committee member	2014 Spring
Applied Physics	director of graduate admissions	2015 Spring
Applied Physics	director of graduate admissions	2016 Spring
Applied Physics	director of graduate admissions	2017 Spring

**Graduate thesis and examination committees**

Committee	Department	Student	Advisor	Year(s)
Oral Exam	Physic	Lei Fang	Alhassid	2003
Special Investigation	Applied Physics	Blair Connelley	Long	2003-2004
Ph.D. Thesis	Electrical Eng.	Wenyong Wang	Reed	2004
Special Investigation	Applied Physics	Shruti Mohanty	—	2004
Area Exam	Applied Physics	Huiqiong Wang	Henrich	2004
Oral Exam	Physics	Minghao Shen	Schoelkopf	2004
Oral Exam	Physics	Yuan Huang	Alhassid	2004
Ph.D. Thesis	Physics	Lei Fang	Alhassid	2005
Ph.D. Thesis	Physics	Minghao Shen	Schoelkopf	2005
Special Investigation	Electrical Eng.	Xiao Pan	Ma	2005
Oral Exam	Physics	George Mias	Girvin	2005
Special Investigation	Chemical Eng.	Yung-Ruey Yen	Altman	2006
Ph.D. Thesis	Physics	Jun Wang	Altman	2007
Ph.D. Thesis	Applied Physics	Huiqiong Wang	Henrich	2007
Ph.D. Thesis	Applied Physics	Agham Posadas	Ahn	2007
Ph.D. Thesis	Physics	Yuan Huang	Alhassid	2008
Area Exam	Applied Physics	Jarrett Moyer	Henrich	2008
Area Exam	Applied Physics	Yaron Segal	Ahn	2008
Ph.D. Thesis	Chemical Eng.	Fang Fang	Pfefferle	2008-2014
Special Investigation	Applied PHYSICS	Emily Allen	Ahn	2008-2009
Ph.D. Thesis	Physics	Li Ge	Stone	2010
Ph.D. Thesis	Applied Physics	Yaron Segal	Ahn	2011
Ph.D. Thesis	Applied Physics	Jarrett Moyer	Henrich	2011
Special Investigation	Applied Physics	Eric Jin	Ahn	2011-2012
Ph.D. Thesis	Applied Physics	Ankit Disa	Ahn	2012-2016
Ph.D. Thesis	Chemical Eng.	Boris Lukanov	Altman	2012
Area Exam	Applied Physics	Eric Jin	Ahn	2013
Oral Exam	Chemistry	Mikhail Askerka	Batista	2013
Ph.D. Thesis	Mech. Eng. & Mat. Sci	Tianqi Shen	O'Hern	2014
Special Investigation	Applied Physics	Stephen Albright	Ahn	2014
Special Investigation	Mech. Eng. & Mat. Sci.	Zheng Chen	Schwarz	2014
Area Exam	Chemistry	Subhajyoti Chaudhuri	Batista	2015
Area Exam	Mech. Eng. & Mat. Sci	Chao Zhou	Schwarz	2016

**Represented Applied Physics at the Yale Engineering tournament:** with team member Prof. R. Shankar. Sadly, the mechanical engineering team beat us (*February 2006*).

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## 9. SERVICE TO THE BROADER SCIENTIFIC COMMUNITY

Grant review (individual grants, collaborative grants, and panel reviews) for the National Science Foundation, Department of Energy, Army Research Office, Petroleum Research Council, and the Molecular Foundry (Lawrence Berkeley National Laboratory).

Reviewer for a variety of journals including Physical Review Letters, Physical Review B, Nano Letters, Europhysics Letters, Applied Physics Letters, Surface Science, New Journal of Physics, Nature, Nature Communications, etc.

Co-organizer of Focus Session on Computational Nanoscience at the March meeting of the American Physical Society (Session J26 DMP DCOMP) (*March 2009*).

Co-organzier of Symposium on Emergent Electron Transport Properties at Complex Oxide Interfaces at

the Fall MRS 2013 meeting (*November 2013*).

Co-organizer of DMP Focus Session “Complex Oxide Interfaces and Heterostructures” at the APS March meeting 2014 (*March 2014*).

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## 10. BROADER OUTREACH

Continual development of educational web material and actual demonstration kits together with a New Haven high school science teacher (Kenneth Spinka). The aim is to teach basic science and engineering to high school students and teachers and to kindle their interest in these subjects: the vehicle is to explain how modern electronic devices (phones, laptops, hard drives, CD/DVD drives, LEDs, flash drives, transistors) work on the materials science level (*Fall 2008 - present*).

First workshop demonstrating above kits drew ~15 high school teachers to Yale where we had lectures, hands on demonstrations, use of the kits, Q&A, and plenty of pizza (*March 24, 2010*).

Public lecture to Chemistry 21 (high school) students at SCSU introducing them to materials physics, materials science, the ideas behind theoretical studies of materials using fundamental physics, and the impact of such research on science and technology (*March 2012*).

Lecture to summer SCHOLARS students at Yale on nanotechnology in every day devices and the basis for magnetic storage of information (*July 2014*).

Public lecture on “How Things Work: The Nano of Computers” organized by CRISP and Yale Pathways to Science, Davies Auditorium at Yale (*September 23, 2014*).

Advisory board member of the Center for 21<sup>st</sup> Century Skills.

Other local outreach:

Location	Function	Semester
Wilbur Cross High School	Science Fair judge	2005 January
New Haven Science Fair	Judge	2005 March
Sheridan Comm. and Tech. Magnet School	Science Fair judge	2006 January
Riverside Educational Academy	Science Fair judge	2006 January
Sheridan Comm. and Tech. Magnet School	Met with robotics class to discuss careers in science	2006 January
New Haven Science Fair	Judge	2007 March