Travis Sjostrom

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Education

2002–2008	Department of Physics, University of Utah, graduate student. Specialization in condensed matter theory and computation. Thesis - "Electronic Energy Band Calculations in Nano-structures" Supervisor - Daniel C. Mattis Graduated 2008, Ph.D.
1997-2002	University of Utah, undergraduate student. Graduated 2002, B.S. Physics.

Experience & Skills

2013-Present	Postdoctoral Associate, Theoretical Division, T-5, Los Alamos National Laboratory Orbital-free DFT theory and code development for molecular dynamics simulations and average atom models, including time-dependent orbital-free and beyond Born-Oppenheimer formulations.
2009-2012	Postdoctoral Associate, Quantum Theory Project, University of Florida Research and development of DFT methods for warm dense matter, including exchange-correlation and orbital-free kinetic energy functionals, and pseudopotentials. Ran and modified various DFT programs, wrote MPI thermal *ab initio* and DFT programs, established and maintained group website.
2004–2008	Research Assistant, University of Utah Thesis - "Electronic Energy Band Calculations in Nano-structures:" Density functional theory calculations for a semiconducting quasi-2D antidot nano-array, as high temperature superconductor model, finding different magnetic ground state depending on geometry and also on an electron filling factor. 2D Hubbard and t-J model comparisons on small clusters.
Jun 2005–Jul 2005	Studied computational physics, including DFT and application to nano-structures at Brookhaven National Laboratory. Continued collaboration through 2008.
2003–2004 & 2005–2008	Teaching Assistant, Dept. of Physics, University of Utah Courses included physics for scientists and engineers, honors introductory physics, graduate statistical mechanics.
Skills	Experience with various DFT codes: Vasp, Q-espresso, Abinit, Siesta, and Profess (orbital-free), including making modifications to them. From scratch code development for *ab initio* wave-function, DFT, and other calculations. Programming: C, C++, Fortran languages utilizing MPI. Scripting: BASH and others.

Publications

Gradient corrections to the exchange-correlation free energy, T. Sjostrom and J. Daligault, *Phys. Rev. B* 90, 155109 (2014).

Fast and accurate quantum molecular dynamics of dense plasmas across temperature regimes, T. Sjostrom and J. Daligault, *Phys. Rev. Lett.* 113, 155006 (2014).

Finite-temperature orbital-free DFT molecular dynamics: coupling Profess and Quantum Espresso, V.V. Karasiev, T. Sjostrom, and S.B. Trickey, *Comput. Phys. Commun.* 185, 3240 (2014).

Accurate homogeneous electron gas exchange-correlation free energy for local spin-density calculations, V.V. Karasiev, T. Sjostrom, J.Dufty, and S.B. Trickey, *Phys. Rev. Lett.* 112, 076403 (2014).

Nonlocal orbital-free noninteracting free-energy functional for warm dense matter, T. Sjostrom and J. Daligault, *Phys. Rev. B* 88, 195103 (2013).

Uniform electron gas at finite temperatures, T. Sjostrom and J. Dufty, *Phys. Rev. B* 88, 115123 (2013).

Innovations in Finite-Temperature Density Functionals, V.V. Karasiev, T. Sjostrom, D.Chakraborty, J.W. Dufty, F.E. Harris, K. Runge, and S.B. Trickey, chapter in *Frontiers and Challenges in Warm Dense Matter*, Lecture Notes in Computational Science and Engineering, Vol. 96, F. Graziani et al. eds., (Springer 2014).

Generalized Gradient Approximation Non-interacting Free Energy Functionals for Orbital-free Density Functional Calculations, V.V. Karasiev, T. Sjostrom, and S.B. Trickey, *Phys. Rev. B* 86, 115101 (2012).

Comparison of Density Functional approximations and the Finite-temperature Hartree-Fock Approximation in Warm Dense Lithium, V.V. Karasiev, T. Sjostrom, and S.B. Trickey, *Phys. Rev. E* 86, 056704 (2012).

Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation, T. Sjostrom, F.E. Harris, and S.B. Trickey, *Phys. Rev. B* 85, 045125 (2012).

Electronic Properties of Thin Film Periodic Nanostructures, T. Sjostrom, D. C. Mattis, W.-G. Yin and W. Ku, *J. Comput. Theor. Nanosci.* Vol. 6, pp 403-417 (2009).

Electronic Energy Band Calculations in Nano-structures, T. Sjostrom, Thesis, University of Utah (2008).

Bloch's Theorem in Nanoarchitectures, D. C. Mattis and T. Sjostrom, *Mod. Phys. Lett. B,* Vol. 20, pp 501-513 (2006).

References

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Wei Ku, Professor of Physics
Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Bldg 510 Upton, NY 11973-5000
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Daniel C. Mattis, Professor of Physics
Department of Physics, University of Utah, 115 S 1400 E Rm 201, Salt Lake City, UT 84112-0830
Email: mattis@physics.utah.edu Fax: 801-581-4801 Phone: 801-581-3690

Presentations

SCCS 2014 *Santa Fe*

Gradient corrections to the exchange-correlation free energy, T. Sjostrom and J. Daligault.

APS March Meeting 2014 *Denver*

Nonlocal orbital-free density functional theory for warm dense matter, T. Sjostrom and J. Daligault.

Local Density Approximation Exchange-correlation Free-energy Functional, V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey

54th Sanibel Symposium, Feb. 2014 (Invited)

Nonlocal orbital-free density functional theory for warm dense matter.

APS-SCCM 2013 *Seattle*

Finite temperature orbital-free density functional theory MD for warm dense matter systems, T. Sjostrom and J. Daligault.

APS March Meeting 2013 *Baltimore*

Gradient corrections to finite-temperature exchange-correlation functionals, T. Sjostrom and J.W. Dufty.

Finite-temperature orbital-free GGA molecular dynamics for warm dense hydrogen, V.V. Karasiev, T. Sjostrom, S.B. Trickey.

14th Int'l Conf. on the Physics of Non-ideal Plasmas (PNP), Sept. 2012 (Poster) *Rostock*

Finite temperature Hartree-Fock and density functional theory calculations on confined hydrogen systems.

CECAM workshop: Orbital-free approach for high energy density physics, Sept. 2012 (Invited) *Paris*

Exchange-Correlation free energy functionals.

IPAM Computational Methods in High Energy Density Plasmas, Workshop IV: Computational Challenges in Warm Dense Matter, May 2012 (Invited) *UCLA*

Finite-Temperature Hartree-Fock Exchange and Exchange-Correlation Free Energy Functionals.

APS March Meeting 2012 *Boston*

Comparison of Finite Temperature Hartree-Fock and Density Functional Theory for Confined Systems, T. Sjostrom, S.B. Trickey, F.E. Harris.

Density Functional versus Thermal Hartree-Fock Approximations in Warm Dense Lithium, V.V. Karasiev, T. Sjostrom, S.B. Trickey.

Construction of Generalized Gradient Approximation Free Energy Density Functionals, S.B. Trickey, V. Karasiev, T. Sjostrom.

APS DPP 2011 *Salt Lake City*

Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation, T. Sjostrom, F.E. Harris, S.B. Trickey.

APS March Meeting 2011 *Dallas*

All-Electron and Pseudopotential Orbital-Free Density Functional Calculations, V.V. Karasiev, T. Sjostrom, S.B. Trickey.

Contributions to the Non-interacting Free Energy Density Functional, S.B. Trickey, J. Dufty, T. Sjostrom.

Finite-temperature Exchange and Correlation Functionals in Self-Consistent Calculations, T. Sjostrom, V.V. Karasiev, S.B. Trickey.

Reference Calculation of Temperature-dependent Behavior of Confined Many-electron Systems, F.E. Harris, T. Sjostrom.