Dr. Daniel G. Sheppard

Computational Physics
Materials and Physical Data
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Current Research Interests

Equation of State for materials from the solid to the warm dense matter region. Extracting of elastic constants, diffusion constants, viscosity, and optical properties from quantum molecular dynamics simulations.

Development of novel methods for the rational design of compounds with desired target properties. Using alchemical derivatives, energy derivatives with respect to chemical identify, to navigate chemical compound space. The goal being the design of materials integral to energy research: fuel cell catalysts, Li battery materials, photovoltaic materials, and photocatalytic materials.

Computational methods for simulation of long time scale kinetics. Saddle point finding for use with harmonic transition state theory and kinetic monte carlo. Applications include water splitting on TiO_2 for use in H_2 production and lithiation of $FePO_4$ as a battery cathode material.

Characterization methods for critical points on potential energy surfaces. Extensive work on optimization of the nudged elastic band method for use in density function theory codes. Development of a new solid-state nudged elastic band method for finding transition pathways for solid-solid phase transitions.

Skills and Computer Literacy

Methods	nudged-elastic band, solid-state neb, molecular dynamics, transition state theory, velocity-auto-correlation, diffusivity, viscosity, Z-method, alchemical derivatives, transport properties
Optimization	Global Optimization, LBFGS, Quick-min, FIRE, CG
Development	GMAN (python), TSSE (python), VTSTCODE for *VASP* (Fortan 90) VTSTSCRIPTS (perl), PESTO (python)
DFT	*VASP*, CPMD
EOS	OPENSESAME, MAGPIE, CHEETAH

Education

2005-2010	University of Texas, Austin: Ph.D in Theoretical Chemistry Thesis Topic: *Methods for Calculating Chemical Properties in the Condensed Phase.* Thesis Advisor: *Prof. Graeme A. Henkelman*
2001-2005	University of California, Davis: B.S. in Chemistry

Awards

Spring 2011 IPAM (workshop): Postdoctoral Research Fellow, UCLA, Los Angeles

Work Experience

2014-present Staff Scientist, Los Alamos National Laboratory, XCP-5
Research: Equation of State and quantum molecular dynamics
Supervisor: *Dr. Kevin Honnell*

2011-2014 Postdoctoral Research Associate, Los Alamos National Laboratory, T-1
Research: Equation of State and quantum molecular dynamics
Supervisor: *Dr. Joel Kress and Dr. Carl Greeff*

2005-2011 Graduate Research Assistant/ Postdoctoral Fellow, University of Texas at Austin
Research: methods for rational compound design and transition state finding
Supervisor: *Prof. Graeme A. Henkelman*

2008 Visiting Scientist, Sandia National Laboratory, Albuquerque, 1435
Research: rational compound design using alchemical derivatives
Supervisors: *Dr. O. Anatole von Lilienfeld*

2000-2005 Undergraduate Summer Research Assistant, Los Alamos National Laboratory, X-5/P-23
Research: photon transport calculations for underground diagnostics and laser holography
Supervisors: *Dr. Roger W. Brewer, Dr. John S. Sarracino, and Dr. Danny S. Sorenson*

2001-2003 Undergraduate Research Assistant, University of California, Davis
Research: solvent properties of supercritical CO_2
Supervisor: *Prof. Philip G. Jessop*

Talks and Posters

04/2014 Seminar XCP-5, Los Alamos National Laboratory

11/2012 JOWOG 32 mat. Los Alamos National Laboratory

06/2012 Electronic Structure Workshop, Wake Forest

05/2011 IPAM: Materials Design in Chemical Compound Space, UCLA

04/2011 Los Alamos National Laboratory

03/2011 IPAM: Navigating Chemical Compound Space, UCLA

12/2010 EFRC:CST External Advisory Committee Meeting, UT Austin

5/2010 EFRC:CST Density Functional Theory Meeting, Santa Fe, NM

Publications

16. D. Sheppard, S. Mazevet, F. J. Cherne, R. C. Albers, K. Kadau, T. C. Germann, J. D. Kress, and L. A. Collins, "Dynamical and transport properties of liquid gallium at high pressures" *Phys. Rev. E*, **91**, 063101 (2015).

15. D. Sheppard, J. D. Kress, S. Crockett, L. A. Collins, and M. P. Desjarlais, "Combining Kohn-Sham and orbital-free density-functional theory for Hugoniot calculations to extreme pressures" *Phys. Rev. E*, **90**, 063314 (2014).

14. K. Falk, C. McCoy, C. L. Fryer, C. W. Greeff, A. L. Hungerford, D. S Montgomery, D. W. Schmidt, D. G. Sheppard, J. R. Williams, T. R. Boehly, and J. F. Benage, "Temperature measurements of shocked silica aerogel foam" *Phys. Rev. E*, **90**, 033107 (2014).

13. P. Xiao, D. Sheppard, J. Rogal, and G. Henkelman "A Generalized Solid-State Dimer Method" *J. Chem. Phys.*, **140**, 174104 (2014).

12. L. Burakovsky, S. P. Chen, D. L. Preston, and D. G. Sheppard, "Z Methodology for Phase Diagram Studies: Platinum and Tantalum as Examples" *J. Phys.: Conf. Ser.*, **500**, 162001 (2014).

11. Z. D. Pozun, K. Hansen, D. Sheppard, M. Rupp, K-R. Müller, and G. Henkelman, "Optimizing transition states *via* kernel-based machine learning" *J. Chem. Phys.* **136**, 174101 (2012).

10. D. Sheppard, P. Xiao, W. Chemelewski, D. D. Johnson, and G. Henkelman, "A generalized solid-state nudged elastic band method" *J. Chem. Phys.* **136**, 074103 (2012).

9. G. K. P. Dathar, D. Sheppard, K. J. Stevenson, and G. Henkelman, "Calculations of Li-Ion Diffusion in Olivine Phosphates" *Chem. Mater.* **23**, 4032-4037 (2011).

8. D. Sheppard and G. Henkelman, "Paths to which the nudged elastic band converges" *J. Comput. Chem.* **32**, 1769 (2011).

7. B. C. Norris, D. G. Sheppard, G. Henkelman and C. W. Bielawski, "Kinetic and thermodynamic evaluation of the reversible n-heterocyclic carbene - isothiocyanate coupling reaction: applications in latent catalysis" *J. Org. Chem.* **76** (1), 301 (2011).

6. D. Sheppard, "Methods for calculating chemical properties in the condensed phase" *Ph.D Thesis from the University of Texas at Austin*, 1-113 (2010).

5. D. Sheppard, G. Henkelman, and O. A. von Lilienfeld, "Alchemical derivatives of reaction energetics" *J. Chem. Phys.* **133**, 084104 (2010).

4. S.-C. Li, Z. Zhang, D. Sheppard, B. D. Kay, J. M. White, Y. Du, I. Lyubinetsky, G. Henkelman, and Z. Dohnalek, "Intrinsic diffusion of hydrogen on rutile TiO_2(110)" *J. Am. Chem. Soc.* **130**, 9080 (2008).

3. D. Sheppard, R. Terrell, and G. Henkelman, "Optimization methods for finding minimum energy paths." *J. Chem. Phys.* **128**, 134106 (2008).

2. C. D. Ablan, D. Sheppard, E. J. Beckman, M. M. Olmstead, and P. G. Jessop. "Solubility of several analogues of triphenylphosphine in carbon dioxide." *Green Chem.* **7**, 590 (2005).

1. P. G. Jessop, M. M. Olmstead, C. D. Ablan, M. Grabenauer, D. Sheppard, C. A. Eckert, and C. L. Liotta. "Carbon dioxide as a solubility 'switch' for the reversible dissolution of highly fluorinated complexes and reagents in organic solvents: application to crystallization." *Inorg. Chem.* **41**, 3463 (2002).

Teaching Experience

2005-2010	Teaching Assistant, University of Texas at Austin Classes: *Physical Chemistry, Physical Chemistry Laboratory, Computational Chemistry, Freshman Research Initiative*
2004-2005	Teaching Assistant, University of California at Davis Classes: *General Chemistry Laboratory*

Misc.

Citizenship: United States
Erdős Number 3

References: available on request