Jonathan E. Moussa

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Citizenship USA

Research Interests Computational physics, computational materials science, scientific computing, condensed matter physics, electronic structure theory, quantum chemistry, quantum information theory, quantum error correction, quantum simulation, numerical analysis, numerical linear algebra, classical algorithms, quantum algorithms.

Education

The University of California at Berkeley, Berkeley, CA, USA

Ph.D., Physics, May 2008

- Thesis Topic: *Theoretical study of electron-phonon superconductivity*
- Adviser: Professor Marvin L. Cohen

Worcester Polytechnic Institute, Worcester, MA, USA

M.S., Physics, May 2004

- Thesis Topic: *The Schroedinger-Poisson selfconsistency in layered quantum semiconductor structures*
- Adviser: Professor L. Ramdas Ram-Mohan

B.S., Mathematics and Physics, May 2001

Job Experience

Software Scientist July 2018 to present
Molecular Sciences Software Institute, Blacksburg, VA USA

Staff Scientist November 2014 to July 2018
Nonconventional Computing Technologies Department,
Center for Computing Research,
Sandia National Laboratories

Postdoctoral Researcher August 2011 to November 2014
Advanced Device Technologies Department,
Center for Computing Research,
Sandia National Laboratories

Postdoctoral Researcher July 2008 to July 2011
Center for Computational Materials,
Institute for Computational Engineering and Sciences,
The University of Texas at Austin

Graduate Student August 2002 to June 2008
Physics Department,
The University of California at Berkeley

Summer Intern Summers of 2000 and 2002
Air Force Research Laboratory's Sensors Directorate,
Wright Patterson Air Force Base

Programming Consultant August 1998 to June 2002
Quantum Semiconductor Algorithms, Northborough, MA USA

H-index **12** (Google Scholar)

Publications

22. Hardy, W. J., C. T. Harris, Y.-H. Su, Y. Chuang, **J. Moussa**, L. N. Maurer, J.-Y. Li, T.-M. Lu, and D. R. Luhman. Single and double hole quantum dots in strained Ge/SiGe quantum wells. *Nanotechnology* 30:215202 (2019). doi:10.1088/1361-6528/ab061e.

21. Chou, C.-T., N. T. Jacobson, **J. E. Moussa**, A. D. Baczewski, Y. Chuang, C.-Y. Liu, J.-Y. Li, and T. M. Lu. Weak anti-localization of two-dimensional holes in germanium beyond the diffusive regime. *Nanoscale* 10:20559 (2018). doi:10.1039/C8NR05677C.

20. **Moussa, J. E.**. Minimax rational approximation of the Fermi-Dirac distribution. *The Journal of Chemical Physics* 145:164108 (2016). doi:10.1063/1.4965886.

19. **Moussa, J. E.**. Transversal Clifford gates on folded surface codes. *Physical Review A* 94:042316 (2016). doi:10.1103/PhysRevA.94.042316.

18. **Moussa, J. E.**. Quantum circuits for qubit fusion. *Quantum Information and Computation* 16:1113 (2016). arXiv:1512.06132.

17. Parekh, O., J. Wendt, L. Shulenburger, A. Landahl, **J. Moussa**, and J. Aidun. Benchmarking Adiabatic Quantum Optimization for Complex Network Analysis. *Journal of Intelligence Community Research and Development* (2015). arXiv:1604.00319.

16. Gamble, J. K., N. T. Jacobson, E. Nielsen, A. D. Baczewski, **J. E. Moussa**, I. Montaño, and R. P. Muller. Multivalley effective mass theory simulation of donors in silicon. *Physical Review B*, 91:235318 (2015). doi:10.1103/PhysRevB.91.235318.

15. Chandra, R., N. T. Jacobson, **J. E. Moussa**, S. H. Frankel, and S. Kais. Quadratic constrained mixed discrete optimization with an adiabatic quantum optimizer. *Physical Review A*, 90:012308 (2014). doi:10.1103/PhysRevA.90.012308.

14. **Moussa, J. E.**. Cubic-scaling algorithm and self-consistent field for the random-phase approximation with second-order screened exchange. *The Journal of Chemical Physics*, 140:014107 (2014). doi:10.1063/1.4855255.

13. **Moussa, J. E.**, S. M. Foiles, and P. A. Schultz. Simulation and modeling of the electronic structure of GaAs damage clusters. *Journal of Applied Physics*, 113:093706 (2013). doi:10.1063/1.4794164.

12. **Moussa, J. E.**. Comment on "Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning". *Physical Review Letters*, 109:059801 (2012). doi:10.1103/PhysRevLett.109.059801.

11. **Moussa, J. E.**, P. A. Schultz, and J. R. Chelikowsky. Analysis of the Heyd-Scuseria-Ernzerhof density functional parameter space. *The Journal of Chemical Physics*, 136:204117 (2012). doi:10.1063/1.4722993.

10. **Moussa, J. E.**, N. Marom, N. Sai, and J. R. Chelikowsky. Theoretical Design of a Shallow Donor in Diamond by Lithium-Nitrogen Codoping. *Physical Review Letters*, 108:226404 (2012). doi:10.1103/PhysRevLett.108.226404.

9. Marom, N., **J. E. Moussa**, X. Ren, A. Tkatchenko, and J. R. Chelikowsky. Electronic structure of dye-sensitized TiO_2 clusters from many-body perturbation theory. *Physical Review B*, 84:245115 (2011). doi:10.1103/PhysRevB.84.245115.

8. Marom, N., X. Ren, **J. E. Moussa**, J. R. Chelikowsky, and L. Kronik. Electronic structure of copper phthalocyanine from G_0W_0 calculations. *Physical Review B*, 84:195143 (2011). doi:10.1103/PhysRevB.84.195143.

7. **Moussa, J. E.**, J. Noffsinger, and M. L. Cohen. Possible thermodynamic stability and superconductivity of $Be_2B_xC_{1-x}$. *Physical Review B*, 78:104506 (2008). doi:10.1103/PhysRevB.78.104506.

6. **Moussa, J. E.** and M. L. Cohen. Using molecular fragments to estimate electron-phonon coupling and possible superconductivity in covalent materials. *Physical Review B*, 78:064502 (2008). doi:10.1103/PhysRevB.78.064502.

5. **Moussa, J. E.** and M. L. Cohen. Constraints on T_c for superconductivity in heavily boron-doped diamond. *Physical Review B*, 77:064518 (2008). doi:10.1103/PhysRevB.77.064518.

4. **Moussa, J. E.** and M. L. Cohen. Two bounds on the maximum phonon-mediated superconducting transition temperature. *Physical Review B*, 74:094520 (2006). doi:10.1103/PhysRevB.74.094520.

3. Ram-Mohan, L. R., K. H. Yoo, and **J. Moussa**. The Schrödinger-Poisson self-consistency in layered quantum semiconductor structures. *Journal of Applied Physics*, 95:3081 (2004). doi:10.1063/1.1649458.

2. **Moussa, J.**, L. R. Ram-Mohan, A. C. H. Rowe, and S. A. Solin. Response of an extraordinary magnetoresistance read head to a magnetic bit. *Journal of Applied Physics*, 94:1110 (2003). doi:10.1063/1.1576897.

1. **Moussa, J.**, L. R. Ram-Mohan, J. Sullivan, T. Zhou, D. R. Hines, and S. A. Solin. Finite-element modeling of extraordinary magnetoresistance in thin film semiconductors with metallic inclusions. *Physical Review B*, 64:184410 (2001). doi:10.1103/PhysRevB.64.184410.

Unpublished Work

11. **Moussa, J. E.**. Measurement-Based Quantum Metropolis Algorithm. arXiv:1903.01451 (2019).

10. **Moussa, J. E.** and A. D. Baczewski. Assessment of localized and randomized algorithms for electronic structure. arXiv:1812.05264 (2018).

9. L. Shulenburger, A. D. Baczewski, S. M. Foiles, A. E. Wills, N. A. Modine, **J. E. Moussa**, P. A. Schultz, V. Tikare, and A. F. Wright. Next-Generation Electronic Structure Codes. Sandia Technical Report SAND2016-9782 (2016).

8. **Moussa, J. E.**. Linear embedding of free energy minimization. arXiv:1603.05180 (2016).

7. Metodi, T. S. , A. J. Landahl, C. Ryan-Anderson, M. S. Carroll, **J. E. Moussa**, and R. P. Muller. SEQIS Late Start LDRD: Final Report - Robust Quantum Operations. Sandia Technical Report SAND2015-10754 (2015).

6. **Moussa, J. E.** and A. D. Baczewski. Comment on "Self-Averaging Stochastic Kohn-Sham Density-Functional Theory". arXiv:1311.6576 (2013).

5. **Moussa, J. E.**. Comment on "Adiabatic Quantum Algorithm for Search Engine Ranking". arXiv:1310.6676 (2013).

4. **Moussa, J. E.** and P. A. Schultz. Accurate numerical integration of an electron exchange hole with a screened Coulomb interaction. arXiv:1210.8233 (2012).

3. **Moussa, J. E.**. Generalized unitary Bogoliubov transformation that breaks fermion number parity. arXiv:1208.1086 (2012).

2. **Moussa, J. E.**. Approximate diagonalization method for many-fermion Hamiltonians. arXiv:1003.2596 (2010).

1. **Moussa, J. E.**. Perfect algebraic coarsening. arXiv:math/0505157 (2005).

Awarded Grants

1. **Moussa, J. E.** and M. Sarovar. Realizing the Power of Near-Term Quantum Technologies. 0.6 FTE for 2 years. *Sandia National Labs' Laboratory Directed Research and Development Program, Defense Systems and Assessments Mission Area* (2015).

Proposed Grants

1. **Moussa, J. E.**. Random phase approximation: models and algorithms for electron correlation. *Basic Energy Sciences, DOE Early Career Research Program* (2014).

Invited Talks

5. **Moussa, J. E.**. Local reduction of Hermitian eigenproblems. *2017 Meeting of the International Linear Algebra Society* (July 24, 2017).
4. **Moussa, J. E.**. Designing shallow donors in diamond. *March Meeting of the American Physical Society* (March 4, 2015).
3. **Moussa, J. E.**. Interdisciplinary Perspectives on Electronic Structure Theory. *Scuseria research group, Rice University* (January 8, 2014).
2. **Moussa, J. E.**. Eigensolvers in Condensed Matter Physics, Condensed Matter Physics in Eigensolvers. *Computer Science Research Institute, Sandia National Laboratories* (March 29, 2011).
1. Chelikowsky, J. R. and **J. E. Moussa**. Algorithms for the Quantum Modeling of the Properties of Nanocrystals, Nanofilms, and Nanowires. *SIAM Conference on Computational Science and Engineering* (March 4, 2009).

Contributed Talks

16. **Moussa, J. E.**. Testing, analysis, and refinement of the quantum Metropolis algorithm. *March Meeting of the American Physical Society* (March 5, 2019).
15. **Moussa, J. E.**. Localized and Randomized Algorithms for Electronic Structure. *March Meeting of the American Physical Society* (March 7, 2018).
14. **Moussa, J. E.**. Transversal Clifford gates on folded surface codes. *March Meeting of the American Physical Society* (March 16, 2017).
13. **Moussa, J. E.**. Convex Lower Bounds for Free Energy Minimization. *March Meeting of the American Physical Society* (March 16, 2016).
12. **Moussa, J. E.**. Quantum Simulation: Classical Algorithms Versus Analog Simulators. *March Meeting of the American Physical Society* (March 3, 2015).
11. **Moussa, J. E.**. Maximum entropy quantum simulation. *XXVI IUPAP Conference on Computational Physics* (August 13, 2014).
10. **Moussa, J. E.**. Acceleration of screened-exchange density-functional calculations with approximate differential overlap. *March Meeting of the American Physical Society* (March 4, 2014).
9. **Moussa, J. E.**. Cubic-scaling algorithm and self-consistent mean field for the random-phase approximation with second-order screened exchange. *March Meeting of the American Physical Society* (March 18, 2013).
8. **Moussa, J. E.**, P. A. Schultz, and J. R. Chelikowsky. Retrofit of the HSE density functional. *March Meeting of the American Physical Society* (February 27, 2012).
7. **Moussa, J. E.** and J. R. Chelikowsky. Size-dependence of electronic and optical properties of armchair graphene nanoislands. *March Meeting of the American Physical Society* (March 23, 2011).

6. **Moussa, J. E.** and J. R. Chelikowsky. The Truncated Eigenfermion Decomposition applied to the Hubbard model. *March Meeting of the American Physical Society* (March 15, 2010).

5. **Moussa, J. E.** and J. R. Chelikowsky. A Brief Introduction to the Truncated Eigenfermion Decomposition. *March Meeting of the American Physical Society* (March 17, 2009).

4. **Moussa, J. E.** and M. L. Cohen. Constraints on T_c for superconductivity in heavily boron-doped diamond. *March Meeting of the American Physical Society* (March 11, 2008).

3. **Moussa, J. E.** and M. L. Cohen. Possibility of superconductivity in high pressure phases of BC_3. *March Meeting of the American Physical Society* (March 6, 2007).

2. **Moussa, J. E.** and M. L. Cohen. Stability Constraints and Local Criteria for the Bounds on T_c of Conventional Superconductors. *March Meeting of the American Physical Society* (March 16, 2006).

1. **Moussa, J. E.** and M. L. Cohen. Compact representation of the Green function of an infinite periodic system. *March Meeting of the American Physical Society* (March 23, 2005).

Patents

1. Hine, D. R., S. A. Solin, T. Zhou, **J. E. Moussa**, L. R. Ram-Mohan, J. M. Sullivan Jr. Method and system for finite element modeling and simulation of enhanced magnetoresistance in thin film semiconductors with metallic inclusions. U.S. Patent #6,937,967 (2005).

Referee for Journals

- *Physical Review B*
- *Physical Review Letters*
- *The Journal of Chemical Physics*
- *Mathematical Reviews*

Awards

- *Salisbury Prize*, Worcester Polytechnic Institute (2001).
- *Employee Recognition Award*, Enceladus: Quantum Computer Benchmarking Team, Sandia National Laboratories (2016).

Teaching Experience

The University of California at Berkeley, Berkeley, CA USA

Graduate Student Instructor **September 2002 to December 2002**

Programming Skills

C, C++, Fortran, Perl, Python, TEX