

Jonathan E. Moussa

CONTACT INFORMATION	Molecular Sciences Software Institute 1880 Pratt Drive, Suite 1100 Blacksburg, VA 24060	<i>Cell:</i> (508) 498-1920 <i>E-mail:</i> jemoussa@vt.edu
CITIZENSHIP	USA	
RESEARCH INTERESTS	Studying the inherent computational complexity of nature through the development of algorithms, software, and hardware for simulations. My early research was focused on electronic structure, numerical analysis, and many-body physics, but my research has since broadened to include error correction and quantum computing.	
EDUCATION	The University of California at Berkeley, Berkeley, CA, USA Ph.D., Physics, May 2008 • Thesis Topic: <i>Theoretical study of electron-phonon superconductivity</i> • Adviser: Professor Marvin L. Cohen Worcester Polytechnic Institute, Worcester, MA, USA M.S., Physics, May 2004 • Thesis Topic: <i>The Schrodinger-Poisson selfconsistency in layered quantum semiconductor structures</i> • 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 (MolSSI), 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	21 (Google Scholar)	

37. A. C. Onyema, C. Dikeocha, **J. Moussa**, and S. M. Loverde, Mapping Allosteric Communication in the Nucleosome with Conditional Activity. [bioRxiv:2025.09.14.676121](https://doi.org/10.26434/chemrxiv-2025-09-14-676121) (2025). [in press, Journal of Chemical Information and Modeling]
36. **J. E. Moussa** and J. J. P. Stewart. MOPAC: An open-source semiempirical molecular orbital program. [MOPAC GitHub repo](https://doi.org/10.26434/chemrxiv-2025-09-14-676121) (2025). [in press, Journal of Open Source Software]
35. Y. Yang, R. Tom, J. A. G. L. Wui, **J. E. Moussa**, and N. Marom. Genarris 3.0: Generating Close-Packed Molecular Crystal Structures with Rigid Press. *Journal of Chemical Theory and Computation* 21:11318 (2025). doi:[10.1021/acs.jctc.5c01080](https://doi.org/10.1021/acs.jctc.5c01080).
34. **J. E. Moussa**. The Enduring Relevance of Semiempirical Quantum Mechanics. *The Journal of Physical Chemistry A* 129:8465 (2025). doi:[10.1021/acs.jpca.5c03425](https://doi.org/10.1021/acs.jpca.5c03425).
33. N. W. Moriarty, **J. Moussa**, and P. D. Adams. Protonation of histidine rings using quantum-mechanical methods. *Acta Crystallographica D: Structural Biology* 80:639 (2024). doi:[10.1107/S2059798324006314](https://doi.org/10.1107/S2059798324006314).
32. C. Bannwarth, B. Hourahine, and **J. Moussa**. Semiempirical methods. **In:** V. Blum *et al.* Roadmap on methods and software for electronic structure based simulations in chemistry and materials. *Electronic Structure* 6:042501 (2024). doi:[10.1088/2516-1075/ad48ec](https://doi.org/10.1088/2516-1075/ad48ec).
31. **J. E. Moussa**. Model selection in atomistic simulation. *The Journal of Chemical Physics* 158:134103 (2023). doi:[10.1063/5.0142248](https://doi.org/10.1063/5.0142248).
30. K. Klymko, C. Mejuto-Zaera, S. J. Cotton, F. Wudarski, M. Urbanek, D. Hait, M. Head-Gordon, K. B. Whaley, **J. Moussa**, N. Wiebe, W. A. de Jong, and N. M. Tubman. Real-time evolution for ultracompact hamiltonian eigenstates on quantum hardware. *PRX Quantum* 3:020323 (2022). doi:[10.1103/PRXQuantum.3.020323](https://doi.org/10.1103/PRXQuantum.3.020323).
29. I. Gayday, A. Teplukhin, **J. Moussa**, and D. Babikov. SpectrumSDT: A program for parallel calculation of coupled rotational-vibrational energies and lifetimes of bound states and scattering resonances in triatomic systems. *Computer Physics Communications* 267:108084 (2021). doi:[10.1016/j.cpc.2021.108084](https://doi.org/10.1016/j.cpc.2021.108084).
28. V. W. Yu, **J. Moussa**, and V. Blum. Accurate Frozen Core Approximation for All-Electron Density-Functional Theory. *The Journal of Chemical Physics* 154:224107 (2021). doi:[10.1063/5.0050296](https://doi.org/10.1063/5.0050296).
27. J. K. Gamble, E. Nielsen, A. Baczewski, **J. E. Moussa**, X. Gao, A. G. Salinger, and R. P. Muller. Advanced Electronic Structure Calculations for Nanoelectronics. (2021) **In:** Shankar S., Muller R., Dunning T., Chen G.H. (eds) *Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile. Springer Series in Materials Science*, vol 284. Springer, Cham. doi:[10.1007/978-3-030-18778-1_18](https://doi.org/10.1007/978-3-030-18778-1_18).
26. V. W. Yu, **J. Moussa**, P. Kus, A. Marek, P. Messmer, M. Yoon, H. Lederer, and V. Blum. GPU-Acceleration of the ELPA2 Distributed Eigensolver for Dense Symmetric and Hermitian Eigenproblems. *Computer Physics Communications* 262:107808 (2021). doi:[10.1016/j.cpc.2020.107808](https://doi.org/10.1016/j.cpc.2020.107808).
25. V. W. Yu, C. Campos, W. Dawson, A. García, V. Havu, B. Hourahine, W. P. Huhn, M. Jacquelin, W. Jia, M. Keceli, R. Laasner, Y. Li, L. Lin, J. Lu, **J. Moussa**, J. E. Roman, A. Vazquez-Mayagoitia, C. Yang, and V. Blum. ELSI – An Open Infrastructure for Electronic Structure Solvers. *Computer Physics Communications* 256:107459 (2020). doi:[10.1016/j.cpc.2020.107459](https://doi.org/10.1016/j.cpc.2020.107459).

24. M. Metcalf, **J. E. Moussa**, W. A. de Jong, and M. Sarovar. Engineered thermalization and cooling of quantum many-body systems. *Physical Review Research* 2:023214 (2020). doi:[10.1103/PhysRevResearch.2.023214](https://doi.org/10.1103/PhysRevResearch.2.023214).
23. **J. E. Moussa** and A. D. Baczewski. Assessment of localized and randomized algorithms for electronic structure. *Electronic Structure* 1:033001 (2019). doi:[10.1088/2516-1075/ab2022](https://doi.org/10.1088/2516-1075/ab2022).
22. W. J. Hardy, 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](https://doi.org/10.1088/1361-6528/ab061e).
21. C.-T. Chou, 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](https://doi.org/10.1039/C8NR05677C).
20. **J. E. Moussa**. Minimax rational approximation of the Fermi-Dirac distribution. *The Journal of Chemical Physics* 145:164108 (2016). doi:[10.1063/1.4965886](https://doi.org/10.1063/1.4965886).
19. **J. E. Moussa**. Transversal Clifford gates on folded surface codes. *Physical Review A* 94:042316 (2016). doi:[10.1103/PhysRevA.94.042316](https://doi.org/10.1103/PhysRevA.94.042316).
18. **J. E. Moussa**. Quantum circuits for qubit fusion. *Quantum Information and Computation* 16:1113 (2016). [arXiv:1512.06132](https://arxiv.org/abs/1512.06132).
17. O. Parekh, 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](https://arxiv.org/abs/1604.00319).
16. J. K. Gamble, N. T. Jacobson, E. Nielsen, A. D. Baczewski, **J. E. Moussa**, I. Montañó, 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](https://doi.org/10.1103/PhysRevB.91.235318).
15. R. Chandra, 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](https://doi.org/10.1103/PhysRevA.90.012308).
14. **J. E. Moussa**. 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](https://doi.org/10.1063/1.4855255).
13. **J. E. Moussa**, 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](https://doi.org/10.1063/1.4794164).
12. **J. E. Moussa**. 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](https://doi.org/10.1103/PhysRevLett.109.059801).
11. **J. E. Moussa**, 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](https://doi.org/10.1063/1.4722993).
10. **J. E. Moussa**, 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](https://doi.org/10.1103/PhysRevLett.108.226404).

9. N. Marom, **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](https://doi.org/10.1103/PhysRevB.84.245115).
8. N. Marom, 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](https://doi.org/10.1103/PhysRevB.84.195143).
7. **J. E. Moussa**, J. Noffsinger, and M. L. Cohen. Possible thermodynamic stability and superconductivity of $\text{Be}_2\text{B}_x\text{C}_{1-x}$. *Physical Review B*, 78:104506 (2008). doi:[10.1103/PhysRevB.78.104506](https://doi.org/10.1103/PhysRevB.78.104506).
6. **J. E. Moussa** 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](https://doi.org/10.1103/PhysRevB.78.064502).
5. **J. E. Moussa** 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](https://doi.org/10.1103/PhysRevB.77.064518).
4. **J. E. Moussa** 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](https://doi.org/10.1103/PhysRevB.74.094520).
3. L. R. Ram-Mohan, 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](https://doi.org/10.1063/1.1649458).
2. **J. Moussa**, 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](https://doi.org/10.1063/1.1576897).
1. **J. Moussa**, 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](https://doi.org/10.1103/PhysRevB.64.184410).

UNPUBLISHED
WORK

16. **J. E. Moussa**. Recursive Magic State Distillation on the Surface Code. [arXiv:2603.05409](https://arxiv.org/abs/2603.05409) (2026). [in review]
15. J. W. Abbot, ... , **J. E. Moussa** , ... , T. Zhu (177 authors). Roadmap on Advancements of the FHI-aims Software Package. [arXiv:2505.00125](https://arxiv.org/abs/2505.00125) (2025). [in review]
14. **J. E. Moussa**. Quantum Metropolis–Hastings algorithm. [arXiv:2503.14970](https://arxiv.org/abs/2503.14970) (2025). [in review]
13. P. Karpov, A. Marek, T. Melson, A. Pöpl, V. W. Yu, B. Hourahine, A. Garcia, W. Dawson, Y. Yao, W. Huhn, **J. Moussa**, S. Hall, R. Maurer, U. Herath, K. Lion, S. Kokott, and V. Blum. Solvers for Large-Scale Electronic Structure Theory: ELPA and ELSI. [arXiv:2502.02460](https://arxiv.org/abs/2502.02460) (2025). [in review]
12. **J. E. Moussa**. Measurement-Based Quantum Metropolis Algorithm. [arXiv:1903.01451](https://arxiv.org/abs/1903.01451) (2022).
11. **J. E. Moussa**. Minimax separation of the Cauchy kernel. [arXiv:1909.06911](https://arxiv.org/abs/1909.06911) (2020).
10. **J. E. Moussa**. Robust decompositions of quantum states. [arXiv:2003.04171](https://arxiv.org/abs/2003.04171) (2020).

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. **J. E. Moussa**. Linear embedding of free energy minimization. [arXiv:1603.05180](#) (2016).
7. T. S. Metodi, 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. **J. E. Moussa** and A. D. Baczewski. Comment on “Self-Averaging Stochastic Kohn-Sham Density-Functional Theory”. [arXiv:1311.6576](#) (2013).
5. **J. E. Moussa**. Comment on “Adiabatic Quantum Algorithm for Search Engine Ranking”. [arXiv:1310.6676](#) (2013).
4. **J. E. Moussa** and P. A. Schultz. Accurate numerical integration of an electron exchange hole with a screened Coulomb interaction. [arXiv:1210.8233](#) (2012).
3. **J. E. Moussa**. Generalized unitary Bogoliubov transformation that breaks fermion number parity. [arXiv:1208.1086](#) (2012).
2. **J. E. Moussa**. Approximate diagonalization method for many-fermion Hamiltonians. [arXiv:1003.2596](#) (2010).
1. **J. E. Moussa**. Perfect algebraic coarsening. [arXiv:math/0505157](#) (2005).

AWARDED GRANTS 1. **J. E. Moussa** 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).

INVITED TALKS 7. **J. E. Moussa**. My technical roadmap for semiempirical electronic structure. *Telluride Workshop on Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications* (July 8, 2024).

6. **J. E. Moussa**. Applications of Rational Function Approximation to Electronic Structure Calculations. *2020 SIAM/CAIMS 2nd Joint Annual Meeting* (July 10, 2020).

5. **J. E. Moussa**. Local reduction of Hermitian eigenproblems. *2017 Meeting of the International Linear Algebra Society* (July 24, 2017).

4. **J. E. Moussa**. Designing shallow donors in diamond. *March Meeting of the American Physical Society* (March 4, 2015).

3. **J. E. Moussa**. Interdisciplinary Perspectives on Electronic Structure Theory. *Scuseria research group, Rice University* (January 8, 2014).

2. **J. E. Moussa**. Eigensolvers in Condensed Matter Physics, Condensed Matter Physics in Eigensolvers. *Computer Science Research Institute, Sandia National Laboratories* (March 29, 2011).

1. J. R. Chelikowsky 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).

23. **J. E. Moussa.** A simple quantum Markov chain Monte Carlo. *March Meeting of the American Physical Society* (March 20, 2025).
22. **J. E. Moussa.** The enduring relevance of semiempirical electronic structure. *2nd PySCF Conference* (January 14, 2025).
21. **J. E. Moussa.** Asymptotic free energy of quantum replicas. *March Meeting of the American Physical Society* (March 7, 2024).
20. **J. E. Moussa.** The future of MOPAC as open-source software. *MOPAC User Meeting* (June 7, 2023).
19. **J. E. Moussa.** Model selection in atomistic simulation. *March Meeting of the American Physical Society* (March 10, 2023).
18. **J. E. Moussa.** MOPAC and semiempirical models: past and future. *March Meeting of the American Physical Society* (March 14, 2022).
17. **J. E. Moussa.** Error bars for Markov chain Monte Carlo data streams. *March Meeting of the American Physical Society* (March 18, 2021).
16. **J. E. Moussa.** Testing, analysis, and refinement of the quantum Metropolis algorithm. *March Meeting of the American Physical Society* (March 5, 2019).
15. **J. E. Moussa.** Localized and Randomized Algorithms for Electronic Structure. *March Meeting of the American Physical Society* (March 7, 2018).
14. **J. E. Moussa.** Transversal Clifford gates on folded surface codes. *March Meeting of the American Physical Society* (March 16, 2017).
13. **J. E. Moussa.** Convex Lower Bounds for Free Energy Minimization. *March Meeting of the American Physical Society* (March 16, 2016).
12. **J. E. Moussa.** Quantum Simulation: Classical Algorithms Versus Analog Simulators. *March Meeting of the American Physical Society* (March 3, 2015).
11. **J. E. Moussa.** Maximum entropy quantum simulation. *XXVI IUPAP Conference on Computational Physics* (August 13, 2014).
10. **J. E. Moussa.** Acceleration of screened-exchange density-functional calculations with approximate differential overlap. *March Meeting of the American Physical Society* (March 4, 2014).
9. **J. E. Moussa.** 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. **J. E. Moussa, P. A. Schultz, and J. R. Chelikowsky.** Retrofit of the HSE density functional. *March Meeting of the American Physical Society* (February 27, 2012).
7. **J. E. Moussa 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. **J. E. Moussa and J. R. Chelikowsky.** The Truncated Eigenfermion Decomposition applied to the Hubbard model. *March Meeting of the American Physical Society* (March 15, 2010).
5. **J. E. Moussa and J. R. Chelikowsky.** A Brief Introduction to the Truncated Eigenfermion Decomposition. *March Meeting of the American Physical Society* (March 17, 2009).

	4. J. E. Moussa and M. L. Cohen. Constraints on T_c for superconductivity in heavily boron-doped diamond. <i>March Meeting of the American Physical Society</i> (March 11, 2008). 3. J. E. Moussa and M. L. Cohen. Possibility of superconductivity in high pressure phases of BC_3. <i>March Meeting of the American Physical Society</i> (March 6, 2007). 2. J. E. Moussa and M. L. Cohen. Stability Constraints and Local Criteria for the Bounds on T_c of Conventional Superconductors. <i>March Meeting of the American Physical Society</i> (March 16, 2006). 1. J. E. Moussa and M. L. Cohen. Compact representation of the Green function of an infinite periodic system. <i>March Meeting of the American Physical Society</i> (March 23, 2005).
PATENTS	1. D. R. Hine, 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).
AWARDS	• <i>Salisbury Prize</i>, Worcester Polytechnic Institute (2001). • <i>Employee Recognition Award</i>, Enceladus: Quantum Computer Benchmarking Team, Sandia National Laboratories (2016).
TEACHING EXPERIENCE	The University of California at Berkeley, Berkeley, CA USA <i>Graduate Student Instructor</i> September 2002 to December 2002
MENTORING EXPERIENCE	12 fellows mentored in the MolSSI Software Fellowship Program
ORGANIZING EXPERIENCE	MOPAC User Meeting (June 7, 2023).
OPEN SOURCE SOFTWARE	Primary maintainer of the Molecular Orbital PACkage (MOPAC).
PROGRAMMING SKILLS	C, C++, Fortran, Python, $\text{\TeX}$