Publications and Published Codes
Samuel B. Trickey
Current as of: 14 August 2025

Publications

1. "Peculiarities of the Structure and Scaling of the Want-Teter Kinetic Energy Density Functional", Liang Sun, S.B. Trickey, Tun Sheng Tan, Valeria Rios-Vargas, Mohan Chen, Wenhui Mi, Xuecheng Shao, and Michele Pavanello, in preparation for Chem. Phys. Lett.

2. "DFT-MD, KS, and OF", Mohan Chen, Aurora Pribram-Jones, François Soubiran, and S.B. Trickey, Chapter 2 of *Warm Dense Matter Roadmap*, Frank Graziani, David Riley, and Jan Vorberger, eds., Plasma Physics and Controlled Fusion, submitted 25 April 2025 (invited).

3. "Uniform Electron Gas", Tobias Dornheim, Valentin Karasiev, Shigenori Tanaka, and S.B. Trickey, Chapter 14 of *Warm Dense Matter Roadmap*, Frank Graziani, David Riley, and Jan Vorberger, eds., in preparation for Plasma Physics and Controlled Fusion, submitted 25 April 2025 (invited).

4. "Performance Improvement of a De-orbitalized Exchange-Correlation Functional", Héctor Francisco R., Bishal Thapa, S.B. Trickey, and A.C. Cancio, in preparation for Phys. Rev. Mat.

5. "Fully thermal meta-GGA exchange-correlation free-energy density functional", K. Hilleke, V.V. Karasiev, S.B. Trickey, R.M.N. Gosshadze, and S. Hu, Phys. Rev. Mat. **9**, L050801 (2025).

6. "Discovery of Spin-crossover Candidates with Equivariant Graph Neural Networks and Relevance-based Classification", Angel Albavera-Mata, Pawan Prakash, Jason B. Gibson, Eric Fonseca, Sijin Ren, Xiaoguang Zhang, Hai-Ping Cheng, Michael Shatruk, S.B. Trickey, and Richard G. Hennig, J. Chem. Th. Comput. **21**, 3913 (2025).

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8. "Magnetic and Thermochemical Properties of Supramolecular Assemblies as Archetypes of Quantum Materials", Angel Albavera-Mata, Shuanglong Liu, Hai-Ping Cheng, Richard G. Hennig, and S.B. Trickey, J. Phys. Chem. A, **128**, 10929 (2024) doi: 10.1021/acs.jpca.4c06723

9. "Removing Orbital Dependence to Improve Exchange-Correlation Functional Accuracy", Héctor Francisco R., A.C. Cancio, and S.B. Trickey, J. Phys. Chem. A, submitted 11 July 2025.

10. "Effective Wang-Teter Kernels for Orbital-free DFT Simulations", Valeria Rios-Vargas, Xuecheng Shao, S.B. Trickey, and Michele Pavanello, Phys. Rev. B, **110**, 085129 (2024)

11. "Reworking the Tao-Mo Exchange-correlation Functional: III. Improved de-orbitalization strategy and faithful de-orbitalization", Héctor Francisco R., A.C. Cancio, and S.B. Trickey, J. Phys. Chem. A, **128**, 6010 (2024) doi:10.1021/acs.jcpa.4c02635

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