



Martin Stoehr

Postdoctoral Scholar, Chemistry

Bio

STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

Publications

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- **Advancing density functional tight-binding method for large organic molecules through equivariant neural networks** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
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2026
- **Locating Ab Initio Transition States via Geodesic Construction on Machine-Learned Potential Energy Surfaces.** *Journal of chemical theory and computation*
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- **Biomolecular dynamics with machine-learned quantum-mechanical force fields trained on diverse chemical fragments.** *Science advances*
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- **Accurate Many-Body Repulsive Potentials for Density-Functional Tight Binding from Deep Tensor Neural Networks** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*

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- **Quantum mechanics of proteins in explicit water: The role of plasmon-like solute-solvent interactions** *SCIENCE ADVANCES*

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- **Theory and practice of modeling van der Waals interactions in electronic-structure calculations** *CHEMICAL SOCIETY REVIEWS*

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- **Quantum-Mechanical Relation between Atomic Dipole Polarizability and the van der Waals Radius** *PHYSICAL REVIEW LETTERS*

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