Stanford

Martin Stoehr

Postdoctoral Scholar, Chemistry

Bio

STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

Publications

PUBLICATIONS

- **libMBD: A general-purpose package for scalable quantum many-body dispersion calculations.** *The Journal of chemical physics*
  Hermann, J., Stohr, M., Goger, S., Chaudhuri, S., Aradi, B., Maurer, R. J., Tkatchenko, A.
  2023; 159 (17)
- **DFTB+, a software package for efficient approximate density functional theory based atomistic simulations (vol 152, 124101, 2020)** *JOURNAL OF CHEMICAL PHYSICS*
  Hourahine, B., Aradi, B., Blum, V., Bonafe, F., Buccheri, A., Camacho, C., Cevallos, C., Deshaye, M. Y., Dumitrica, T., Dominguez, A., Ehlert, S., Elstner, M., van der Heide, et al
  2022; 157 (3): 039901
- **Coulomb interactions between dipolar quantum fluctuations in van der Waals bound molecules and materials** *NATURE COMMUNICATIONS*
  Stoehr, M., Sadhukhan, M., Al-Hamdani, Y. S., Hermann, J., Tkatchenko, A.
  2021; 12 (1): 137
- **Accurate Many-Body Repulsive Potentials for Density-Functional Tight Binding from Deep Tensor Neural Networks** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Stoehr, M., Sandonas, L., Tkatchenko, A.
  2020; 11 (16): 6835-6843
- **Quantum mechanics of proteins in explicit water: The role of plasmon-like solute-solvent interactions** *SCIENCE ADVANCES*
  Stohr, M., Tkatchenko, A.
  2019; 5 (12): eaax0024
- **Theory and practice of modeling van der Waals interactions in electronic-structure calculations** *CHEMICAL SOCIETY REVIEWS*
  Stohr, M., Van Voorhis, T., Tkatchenko, A.
  2019; 48 (15): 4118-4154
- **Quantum-Mechanical Relation between Atomic Dipole Polarizability and the van der Waals Radius** *PHYSICAL REVIEW LETTERS*
  Fedorov, D., Sadhukhan, M., Stoehr, M., Tkatchenko, A.
  2018; 121 (18): 183401
- **Communication: Charge-population based dispersion interactions for molecules and materials** *JOURNAL OF CHEMICAL PHYSICS*
  Stoehr, M., Michelitsch, G. S., Tully, J. C., Reuter, K., Maurer, R. J.
  2016; 144 (15): 151101

- **Dynamics of Spatially Confined Bisphenol A Trimers in a Unimolecular Network on Ag(111)** *NANO LETTERS*
  Lloyd, J. A., Papageorgiou, A. C., Fischer, S., Oh, S., Saglam, O., Diller, K., Duncan, D. A., Allegretti, F., Klappenberger, F., Stoehr, M., Maurer, R. J., Reuter, K., Reichert, et al
  2016; 16 (3): 1884-1889