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Bio

STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

Publications

PUBLICATIONS

- **Detection and Correction of Delocalization Errors for Electron and Hole Polarons Using Density-Corrected DFT.** *The journal of physical chemistry letters*
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- **Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package** *JOURNAL OF CHEMICAL PHYSICS*
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2021; 155 (8)
- **Hidden Hemibonding in the Aqueous Hydroxyl Radical** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
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- **Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
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- **Ab Initio Investigation of the Resonance Raman Spectrum of the Hydrated Electron** *JOURNAL OF PHYSICAL CHEMISTRY B*
Dasgupta, S., Rana, B., Herbert, J. M.
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- **Variational Formulation of the Generalized Many-Body Expansion with Self-Consistent Charge Embedding: Simple and Correct Analytic Energy Gradient for Fragment-Based ab Initio Molecular Dynamics** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
Liu, J., Rana, B., Liu, K., Herbert, J. M.
2019; 10 (14): 3877-3886
- **Analytic gradient for the QM/MM-Ewald method using charges derived from the electrostatic potential: Theory, implementation, and application to ab initio molecular dynamics simulation of the aqueous electron** *JOURNAL OF CHEMICAL PHYSICS*
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