

Stanford

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Bio

STANFORD ADVISORS

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Publications

PUBLICATIONS

- **Simulating the Excited-State Dynamics of Polaritons with Ab Initio Multiple Spawning.** *The journal of physical chemistry. A* Rana, B., Hohenstein, E. G., Martínez, T. J. 2023
- **Correcting pi-delocalisation errors in conformational energies using density-corrected DFT, with application to crystal polymorphs** *MOLECULAR PHYSICS* Rana, B., Beran, G. O., Herbert, J. M. 2022
- **Detection and Correction of Delocalization Errors for Electron and Hole Polarons Using Density-Corrected DFT.** *The journal of physical chemistry letters* Rana, B., Coons, M. P., Herbert, J. M. 2022: 5275-5284
- **Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package** *JOURNAL OF CHEMICAL PHYSICS* Epifanovsky, E., Gilbert, A. B., Feng, X., Lee, J., Mao, Y., Mardirossian, N., Pokhilko, P., White, A. F., Coons, M. P., Dempwolff, A. L., Gan, Z., Hait, D., Horn, et al 2021; 155 (8)
- **Hidden Hemibonding in the Aqueous Hydroxyl Radical** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS* Rana, B., Herbert, J. M. 2021; 12 (33): 8053-8060
- **Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS* Rana, B., Herbert, J. M. 2020; 22 (47): 27829-27844
- **Ab Initio Investigation of the Resonance Raman Spectrum of the Hydrated Electron** *JOURNAL OF PHYSICAL CHEMISTRY B* Dasgupta, S., Rana, B., Herbert, J. M. 2019; 123 (38): 8074-8085
- **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* Holden, Z. C., Rana, B., Herbert, J. M. 2019; 150 (14): 144115