

# Stanford

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## Diptarka Hait

Postdoctoral Scholar, Chemistry

Curriculum Vitae available Online

### Bio

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#### HONORS AND AWARDS

- Stanford Science Fellow, School of Humanities and Science, Stanford University. (07/01/2022-06/30/2025)

#### STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

#### LINKS

- Google Scholar: <https://scholar.google.com/citations?user=R2WrGKMAAAJ&hl=en>
- Stanford Science Fellows Profile: <https://stanfordsciencefellows.stanford.edu/people/diptarka-hait>

### Research & Scholarship

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#### LAB AFFILIATIONS

- Todd Martinez (7/1/2022)

### Publications

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#### PUBLICATIONS

- Understanding ion-transfer reactions in silver electrodissolution and electrodeposition from first-principles calculations and experiments** *CHEMICAL SCIENCE*  
Kang, R., Zhao, Y., Hait, D., Gauthier, J. A., Kempler, P. A., Thurman, K. A., Boettcher, S. W., Head-Gordon, M.  
2024
- Predicting the X-ray Absorption Spectrum of Ozone with Single Configuration State Functions.** *Journal of chemical theory and computation*  
Hait, D., Martínez, T. J.  
2024
- When is a bond broken? The polarizability perspective.** *Angewandte Chemie (International ed. in English)*  
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- Probing C-I bond fission in the UV photochemistry of 2-iodothiophene with core-to-valence transient absorption spectroscopy.** *The Journal of chemical physics*  
Toulson, B. W., Hait, D., Facciala, D., Neumark, D. M., Leone, S. R., Head-Gordon, M., Gessner, O.  
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- **Femtosecond symmetry breaking and coherent relaxation of methane cations via x-ray spectroscopy.** *Science (New York, N.Y.)*  
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- **Ultrafast X-ray Spectroscopy of Intersystem Crossing in Hexafluoroacetylacetone: Chromophore Photophysics and Spectral Changes in the Face of Electron-Withdrawing Groups.** *The journal of physical chemistry. A*  
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- **Jahn-Teller distortion and dissociation of CCl<sub>4+</sub> by transient X-ray spectroscopy simultaneously at the carbon K- and chlorine L-edge (vol 13, pg 9310, 2022) CHEMICAL SCIENCE**  
Ross, A. D., Hait, D., Scutelnic, V., Haugen, E. A., Ridente, E., Balkew, M. B., Neumark, D. M., Head-Gordon, M., Leone, S. R.  
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- **Jahn-Teller distortion and dissociation of CCl<sub>4+</sub> by transient X-ray spectroscopy simultaneously at the carbon K- and chlorine L-edge CHEMICAL SCIENCE**  
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- **Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four JOURNAL OF CHEMICAL THEORY AND COMPUTATION**  
Liang, J., Feng, X., Hait, D., Head-Gordon, M.  
2022; 18 (6): 3460-3473
- **Computing x-ray absorption spectra from linear-response particles atop optimized holes JOURNAL OF CHEMICAL PHYSICS**  
Hait, D., Oosterbaan, K. J., Carter-Fenk, K., Head-Gordon, M.  
2022; 156 (20): 201104
- **Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on PRX QUANTUM**  
Klymko, K., Mejuto-Zaera, C., Cotton, S. J., Wudarski, F., Urbanek, M., Hait, D., Head-Gordon, M., Whaley, K., Moussa, J., Wiebe, N., de Jong, W. A., Tubman, N. M.  
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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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- **Accurate prediction of core-level spectra of radicals at density functional theory cost via square gradient minimization and recoupling of mixed configurations** *JOURNAL OF CHEMICAL PHYSICS*  
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- **Highly Accurate Prediction of Core Spectra of Molecules at Density Functional Theory Cost: Attaining Sub-electronvolt Error from a Restricted Open-Shell Kohn-Sham Approach** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*  
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• **Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*

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• **How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*

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• **Communication: xDH double hybrid functionals can be qualitatively incorrect for non-equilibrium geometries: Dipole moment inversion and barriers to radical-radical association using XYG3 and XYGJ-OS** *JOURNAL OF CHEMICAL PHYSICS*

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• **How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*

Hait, D., Head-Gordon, M.  
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• **A hybrid memory kernel approach for condensed phase non-adiabatic dynamics** *JOURNAL OF CHEMICAL PHYSICS*

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• **Condensed phase electron transfer beyond the Condon approximation** *JOURNAL OF CHEMICAL PHYSICS*

Mavros, M. G., Hait, D., Van Voorhis, T.  
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• **Prediction of Excited-State Energies and Singlet Triplet Gaps of Charge-Transfer States Using a Restricted Open-Shell Kohn-Sham Approach** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*

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2016; 12 (7): 3353-3359