Stanford

Dip Hait

Postdoctoral Scholar, Chemistry

Curriculum Vitae available Online

Bio

HONORS AND AWARDS

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

PROFESSIONAL EDUCATION

- Doctor of Philosophy, University of California Berkeley (2022)
- Bachelor of Science, Massachusetts Institute of Technology (2016)

STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

LINKS

- Google Scholar: https://scholar.google.com/citations?user=R2WrGKMAAAAJ&hl=en
- Stanford Science Fellows Profile: https://stanfordsciencefellows.stanford.edu/people/diptarka-hait

Research & Scholarship

LAB AFFILIATIONS

- Todd Martinez (7/1/2022)

Publications

PUBLICATIONS

- **Jahn-Teller distortion and dissociation of CCl4+ 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.
  2022
- **Jahn-Teller distortion and dissociation of CCl4+ by transient X-ray spectroscopy simultaneously at the carbon K- and chlorine L-edge** *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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- **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*
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- **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.
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- **Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy.** *The journal of physical chemistry letters*
  Cunha, L. A., Hait, D., Kang, R., Mao, Y., Head-Gordon, 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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- **Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulson-Fischer point in bond dissociation?** *JOURNAL OF CHEMICAL PHYSICS*
  Cunha, L. A., Lee, J., Hait, D., McCurdy, C., Head-Gordon, M.
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- **Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition** *JOURNAL OF CHEMICAL PHYSICS*
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- **Two-Coordinate Iron(I) Complexes on the Edge of Stability: Influence of Dispersion and Steric Effects** *ORGANOMETALLICS*
  Witzke, R. J., Hait, D., Head-Gordon, M., Tilley, T.
  2021; 40 (11): 1758-1764

- **Orbital Optimized Density Functional Theory for Electronic Excited States** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Hait, D., Head-Gordon, M.
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- **Too big, too small, or just right? A benchmark assessment of density functional theory for predicting the spatial extent of the electron density of small chemical systems** *JOURNAL OF CHEMICAL PHYSICS*
  Hait, D., Liang, Y., Head-Gordon, M.
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- **Electron-Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Yoneda, Y., Mora, S., Shee, J., Wadsworth, B. L., Arsenault, E. A., Hait, D., Kodis, G., Gust, D., Moore, G. F., Moore, A. L., Head-Gordon, M., Moore, T. A., Fleming, et al
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- **The Ground State Electronic Energy of Benzene** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
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- **Bimetallic Mechanism for Alkyne Cyclotrimerization with a Two-Coordinate Fe Precatalyst** *ACS CATALYSIS*
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- **Excited State Orbital Optimization via Minimizing the Square of the Gradient: General Approach and Application to Singly and Doubly Excited States via Density Functional Theory** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
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- **Beyond the Coulson-Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
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- **What Levels of Coupled Cluster Theory Are Appropriate for Transition Metal Systems? A Study Using Near-Exact Quantum Chemical Values for 3d Transition Metal Binary Compounds** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
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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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