Diptarka Hait

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Experience

Stanford University; Stanford, CA, USA. Jul 2022–Current
Stanford Science Fellow | Postdoctoral Scholar
Research Advisor: Professor Todd Martinez.

Education

University of California, Berkeley; Berkeley, CA, USA. Aug 2016–May 2022
Ph.D. in Physical Chemistry. GPA: 4.0/4.0.
Thesis: A Density Functional Odyssey Beyond Ground State Energies.
Research Advisor: Professor Martin Head-Gordon

Massachusetts Institute of Technology; Cambridge, MA, USA. Sept 2012–Jun 2016
Bachelor of Science in Chemistry and Physics. GPA: 5.0/5.0.
Thesis: Theoretical Studies on the Properties and Dynamics of Electronic Excited States
Research Advisor: Professor Troy Van Voorhis

Publications as First or Second Author
(* indicates authors contributed equally)

1. Ross, A.D.*; **Hait, D.***; Scutelnic, V.; Haugen, E.A.; Ridente, E.; Balkew, M.B.; Neumark, D.M.; Head-Gordon, M. ; Leone, S.R. "Jahn-Teller Distortion and Dissociation of CCl_4^+ by Transient X-ray Spectroscopy Simultaneously at the Carbon K- and Chlorine L-Edge." *Chem. Sci.,* **13,** 9310-9320. 2022.
2. **Hait, D**.; Oosterbaan, K.J.; Carter-Fenk, K.; Head-Gordon, M. "Computing x-ray absorption spectra from linear-response particles atop optimized holes." *J. Chem. Phys.,* **156,** 201104. 2022.
3. Cunha, L.A.*; **Hait, D**.*; Kang, R.; Mao, Y. Head-Gordon, M. "Relativistic Orbital Optimized Density Functional Theory for Accurate Core-Level Spectroscopy. *J. Phys. Chem. Lett.,* **13**, 3438–3449. 2022.
4. **Hait, D**.; Head-Gordon, M. "Orbital Optimized Density Functional Theory for Electronic Excited States." *J. Phys. Chem. Lett.,* **12**, 4517-4529. 2021.
5. Witzke, R.J.; **Hait, D.**; Head-Gordon, M.; Tilley, T.D. "Two-Coordinate Iron(I) Complexes on the Edge of Stability: Influence of Dispersion and Steric Effects." *Organometallics,* **40,** 1758–1764. 2021.
6. **Hait, D**.*; Liang, Y.H.*; Head-Gordon, M. "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." *J. Chem. Phys.,* **154**, 074109. 2021.
7. Rettig, A.*; **Hait, D**.*; Bertels, L.W.; Head-Gordon, M. "Third order Møller-Plesset theory made more useful? The role of density functional theory orbitals" *J. Chem. Theory Comput.,* **16**, 7473-7489. 2020.
8. **Hait, D.**; Haugen, E.A.; Yang, Z.; Oosterbaan, K.J.; Leone, S.R.; Head-Gordon, M. "Accurate prediction of core-level spectra of radicals at density functional theory cost via square gradient minimization and recoupling of mixed configurations." *J. Chem. Phys.,* **153**, 134108. 2020.
9. Witzke, R.J.; **Hait, D.**; Chakarawet, K.; Head-Gordon, M.; Tilley, T.D. "Bimetallic mechanism for alkyne cyclotrimerization with a two-coordinate Fe precatalyst." *ACS Catal.,* **10**, 7800–7807. 2020.
10. Levine, D.S.; **Hait, D**.; Tubman, N.M.; Lehtola, S.; Whaley, K.B.; Head-Gordon, M. "CASSCF with Extremely Large Active Spaces using the Adaptive Sampling CI Method." *J. Chem. Theory Comput.*, **16**, 2340-2354. 2020.
11. **Hait, D.**; Head-Gordon, M. "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." *J. Chem. Theory Comput.*, **16**, 1699-1710. 2020.
12. **Hait, D**.; Head-Gordon, M. "Highly Accurate Prediction of Core Spectra of Molecules at Density Functional Theory Cost: Attaining sub Sub-electronvolt Error from a Restricted Open-Shell Kohn-Sham Approach." *J. Phys. Chem. Lett.*, **11**, 775-786. 2020.
13. **Hait, D**.*; Rettig, A.*; Head-Gordon, M. "Beyond the Coulson-Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations" *Phys. Chem. Chem. Phys.*, **21**, 21761-21775. 2019. *Selected as a PCCP HOT Article, and as Editor's choice.*

14. **Hait, D.**; Tubman, N.M.; Levine, D.S.; Whaley, K.B.; Head-Gordon, M. "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." *J. Chem. Theory Comput.*, **15**, 5370-5385. 2019.
15. Fang, J.; **Hait, D.**; Head-Gordon, M.; Chang, M.C.Y. "Chemoenzymatic platform for synthesis of chiral organofluorines based on type II aldolases." *Angew. Chem. Int. Ed.*, **58**, 11841-11845. 2019.
16. **Hait, D.***; Rettig, A.*; Head-Gordon, M. "Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H_2" *J. Chem. Phys.*, **150**, 094115. 2019. *Selected as Featured article.*
17. **Hait, D.**; Head-Gordon, M. "Delocalization errors in density functional theory are essentially quadratic in fractional electron number." *J. Phys. Chem. Lett.*, **9**, 6280-6288. 2018.
18. **Hait, D.**; Head-Gordon, M. "How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry." *Phys. Chem. Chem. Phys.*, **20**, 19800-19810. 2018. *Selected as a PCCP HOT Article.*
19. **Hait, D.**; Head-Gordon, M. "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." *J. Chem. Phys.*, **148**, 171102. 2018. *Selected as Editor's Pick.*
20. **Hait, D.**; Head-Gordon, M. "How accurate is density functional theory at predicting dipole moments? An assessment using a new database of 200 benchmark values." *J. Chem. Theory Comput.*, **14**, 1969-1981. 2018.
21. **Hait, D.**; Mavros, M.; Van Voorhis, T. "A hybrid memory kernel approach for condensed phase non-adiabatic dynamics." *J. Chem. Phys.*, **147**, 014108. 2017.
22. Mavros, M.; **Hait, D.**; Van Voorhis, T. "Condensed phase electron transfer beyond the Condon approximation." *J. Chem. Phys.*, **145**, 214105. 2016.
23. **Hait, D.**; Zhu, T.; McMahon, D. P.; Van Voorhis, T. "Prediction of excited state energies and singlet-triplet gaps of charge-transfer states using a Restricted Open-Shell Kohn-Sham approach." *J. Chem. Theory Comput.*, **12**, 3353-3359. 2016.

Publications as Contributing Author

1. Liang, J. *et.al.* "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." *J. Chem. Theory Comput.* **Accepted**. 2022.
2. Klymko, K. *et.al.* "Real time evolution for ultracompact Hamiltonian eigenstates on quantum hardware." *Phys. Rev. X Quantum.* **3**, 020323. 2022.
3. Epifanovsky, E. *et.al.* "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package." *J. Chem. Phys.* **155**, 084801. 2021.
4. Cunha, L.A. *et.al.* "Exploring Spin Symmetry-Breaking Effects for Static Field Ionization of Atoms: Is There an Analog to the Coulson-Fischer Point in Bond Dissociation?" *J. Chem. Phys.* **155**, 014309. 2021.
5. Shee, J. *et.al.* "Revealing the Nature of Electron Correlation in Transition Metal Complexes with Symmetry-Breaking and Chemical Intuition." *J. Chem. Phys.* **154**, 194109. 2021.
6. Yoneda, Y. *et.al.* "Electron-nuclear dynamics accompanying proton-coupled electron transfer." *J. Am. Chem. Soc.*, **143**, 3104-3112. 2021.
7. Eriksen, J.J. *et.al.* "The Ground State Electronic Energy of Benzene." *J. Phys. Chem. Lett.*, **11**, 8922-8929. 2020.
8. Oosterbaan, K.J. *et.al.* "Generalized Single Excitation Configuration Interaction: An Investigation into the Impact of the Inclusion of Non-Orthogonality on the Calculation of Core-Excited States." *Phys. Chem. Chem. Phys.*, **22**, 8182-8192. 2020.
9. Tubman, N.M. *et.al.* "Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method." *J.Chem.Theory Comput.* **16**, 2139-2159. 2020.
10. Lucas, M. *et.al.* "Bimolecular reaction dynamics in the phenyl-silane system: Exploring the prototype of a radical substitution mechanism." *J. Phys. Chem. Lett.*, **9**, 5135-5142. 2018.

Preprints

(* indicates authors contributed equally)

1. Baek, U.; **Hait, D.**; Shee, J.; Leimkuhler, O.; Huggins, W.J.; Stetina, T.F.; Head-Gordon, M.; Whaley, K.B. "Say NO to Optimization: A Non-Orthogonal Quantum Eigensolver." *arXiv:2205.09039*.
2. Tubman, N.M. *et.al.* "An efficient deterministic perturbation theory for selected configuration interaction methods." *arXiv:1808.02049*.
3. Tubman, N.M. *et.al.* "Postponing the orthogonality catastrophe: efficient state preparation for electronic structure simulations on quantum devices." *arXiv:1809.05523*.

Selected Talks

1. **Hait, D**.; Head-Gordon, M. "Orbital optimized density functional theory for core-level spectroscopy." PHYS Symposium on The Synergy of Theory and Experiment: A Symposium in Honor of Prof. John F. Stanton. **ACS San Diego 2022**.
2. **Hait, D**.; Head-Gordon, M. "Cheap and reliable optimization of excited state orbitals with the Square Gradient Minimization (SGM) approach." Division of Chemical Physics. **APS 2021**.
3. **Hait, D**.; Rettig, A.; Head-Gordon, M. "Can unrestricted Kohn-Sham DFT qualitatively describe dissociation of H_2?" PHYS Symposium on Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer. **ACS San Diego 2019**.
4. **Hait, D**.; Tubman, N.M.; Levine, D.S.; Whaley, K.B. ; Head-Gordon, M. "Quantum chemistry of strongly correlated transition metal systems with the Adaptive Sampling Configuration Interaction Self Consistent Field (ASCI-SCF) method." COMP Symposium on Transition Metal Chemistry & Spectroscopy with Quantum Chemistry. **ACS San Diego 2019**.

Teaching

(as Teaching Assistant)

- **Berkeley:** Chem 295 (Computational Quantum Chemistry: Graduate level), Chem 120B (Physical Chemistry II), Chem 4A (General Chemistry for Chemistry majors).
- **MIT:** 10.637 (Quantum Chemical Simulations: Graduate level), 5.61 (Physical Chemistry I).

Awards

Stanford Science Fellow: Postdoctoral fellowship. 2022-2025
Pimentel Research Award: UC Berkeley Department of Chemistry, for graduate research. 2022
IBM-Zerner Graduate Student Award: 61st Sanibel Symposium. 2022
Graduate Award in Theoretical Chemistry: Finalist. ACS Division of Physical Chemistry. 2021
Reaxys PhD Prize: Finalist. 2020
CCG Graduate Research Excellence Award: ACS Division of Computers in Chemistry. 2019
Berkeley Fellowship: UC Berkeley (for graduate studies). 2016–2019
James R. Killian, Jr. (1926) Scholarship: MIT (for undergraduate studies). 2012–2016
Alpha Chi Sigma Award 2016
MIT Chemistry Department, for outstanding achievement in scholarship, research, and service.
F.D. Greene Teaching Award: MIT Chemistry Department. 2016
Phi Beta Kappa Honor Society: Elected to the Xi Chapter (Massachusetts). 2016
Sigma Pi Sigma Physics Honor Society: Elected to the MIT Chapter. 2016
Sophomore Achievement Award: MIT Chemistry Department. 2014
Freshman Achievement Award: MIT Chemistry Department. 2013
International Chemistry Olympiad: Gold medalist (2011, 2012), Silver medalist (2010).

Mentorship

Graduate Students: Adam Rettig, Juan Arias-Martinez, Richard Kang, Leonardo dos Anjos Cunha, Hengyuan Shen.
Undergraduate Students: Yu Hsuan Liang (currently PhD student at Columbia University).

Professional Activities

Peer Reviewer: *J. Phys. Chem. Lett.; J. Chem. Theory Comput.; Phys. Chem. Chem. Phys.; J. Chem. Phys.; Mol. Phys.; J. Phys. Chem. A; Macromolecules*
Student Commitee for Faculty Hiring (UC Berkeley): Member (2019).
Transfer Student Mentorship Program (UC Berkeley): Planning committee, mentor (2020).
Chemistry Graduate Student Life Committee (UC Berkeley): Member (2016–2019).
MIT Undergraduate Chemistry Association: Member (2014–2016), Co-president (2015-2016).