Diptarka Hait

Contact Information

48 Gilman Hall
University of California, Berkeley

E-mail: diptarka@berkeley.edu
Webpage: https://diphait.wordpress.com/

Education

University of California, Berkeley; Berkeley, CA, USA. 2016–current
Candidate for Ph.D. in Physical Chemistry. GPA: 4.0/4.0.
Advisor: Professor Martin Head-Gordon

Massachusetts Institute of Technology; Cambridge, MA, USA. 2012–2016
Bachelor of Science in Chemistry and Physics. GPA: 5.0/5.0.
Research Advisor: Professor Troy Van Voorhis

Publications (First or Second Author)

1. 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.* **Accepted**. 2020.
2. 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 (4)**, 2340-2354. 2020.
3. **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 (3)**, 1699-1710. 2020.
4. **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 (3)**, 775-786. 2020.
5. **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 (39)**, 21761-21775. 2019. *D.H. and A.R. contributed equally.
Selected in the 2019 PCCP HOT Articles collection and as Editor's choice.
6. **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(10)**, 5370-5385. 2019.
7. 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(34)**, 11841-11845. 2019.
8. **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 (9)**, 094115. 2019. *D.H. and A.R. contributed equally.
Selected as Featured article.
9. **Hait, D**.; Head-Gordon, M. "Delocalization errors in density functional theory are essentially quadratic in fractional electron number." *J. Phys. Chem. Lett.*, **9 (21)**, 6280-6288. 2018.
10. **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 (30)**, 19800-19810. 2018. *Selected in the 2018 PCCP HOT Articles collection.*
11. **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 (17)**, 171102. 2018.
Selected as Editor's Pick.
12. **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 (4)**, 1969-1981. 2018.
13. **Hait, D**.; Mavros, M.; Van Voorhis, T. "A hybrid memory kernel approach for condensed phase non-adiabatic dynamics." *J. Chem. Phys.*, **147 (1)**, 014108. 2017.
14. Mavros, M.; **Hait, D**.; Van Voorhis, T. "Condensed phase electron transfer beyond the Condon approximation." *J. Chem. Phys.*, **145 (21)**, 214105. 2016.

15. **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 (7)**, 3353-3359. 2016.

Publications (Contributing Author)

1. Oosterbaan, K.J.; White, A.F.; **Hait, D.**; Head-Gordon, M. "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 (15)**, 8182-8192. 2020.
2. Tubman, N.M.; Freeman, C.D.; Levine, D.S.; **Hait, D.**; Head-Gordon, M. ; Whaley, K.B. "Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method." *J. Chem. Theory Comput.* **16 (4)**, 2139-2159. 2020.
3. Lucas, M.; Thomas, A.M.; Yang, T.; Kaiser, R.I.; Mebel, A.M.; **Hait, D.**; Head-Gordon, M. "Bimolecular reaction dynamics in the phenyl-silane system: Exploring the prototype of a radical substitution mechanism." *J. Phys. Chem. Lett.*, **9 (17)**, 5135-5142. 2018.

Preprints

1. **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." *arXiv:2006.10181.*
2. Tubman, N.M.; Levine, D.S.; **Hait, D.**; Head-Gordon, M.; Whaley, K.B. "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.*

Recent Talks

1. **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**.
2. **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**.
3. **Hait, D.**; Head-Gordon, M. "Characterizing density and delocalization errors in DFT." COMP Symposium on Recent Advances in DFT & TDDFT. **ACS Boston 2018**.

Teaching

Teaching Assistant

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

Awards

CCG Graduate Research Excellence Award: ACS COMP Division. 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).

Professional Activities

Peer Reviewer: *J. Chem. Theory Comput.; Phys. Chem. Chem. Phys.; Mol. Phys.*
Student Commitee for Faculty Hiring (UC Berkeley): Member (2019).
Chemistry Graduate Student Life Committee (UC Berkeley): Member (2016–present).
MIT Undergraduate Chemistry Association: Member (2014–2016), Co-president (2015-2016).