Diptarka Hait

Contact Information

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Education

University of California, Berkeley; Berkeley, CA, USA. 2016–current
Candidate for Ph.D. in Physical Chemistry. GPA: 4.0/4.0.

Massachusetts Institute of Technology; Cambridge, MA, USA. 2012–2016
Bachelor of Science in Chemistry and Physics. GPA: 5.0/5.0.

Research Experience

Advisor: Professor Martin Head-Gordon 2016–current

- Project I: Development of density functionals for quantum chemistry.
- Project II: Development of orbital optimized excited state techniques.
- Project III: Development of perturbation theories for selected CI algorithms.

Advisor: Professor Troy Van Voorhis 2013–2016

Publications

1. **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.* 2020.
2. **Hait, D**.; Head-Gordon, M. "Highly Accurate Prediction of Core Spectra of Molecules at Density Functional Theory Cost: Attaining sub eV Error from a Restricted Open-Shell Kohn-Sham Approach." *J. Phys. Chem. Lett.*, **11**, 775-786. 2020.
3. **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. * D.H. and A.R. contributed equally.
Selected in the 2019 PCCP HOT Articles collection.
4. **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.
5. 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.
6. **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.
7. **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.
8. 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.
9. **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.
10. **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.

11. **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.
12. **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.
13. Mavros, M.; **Hait, D**.; Van Voorhis, T. "Condensed phase electron transfer beyond the Condon approximation." *J. Chem. Phys.*, **145 (21)**, 214105. 2016.
14. **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.

Preprints and Works in preparation

1. 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." *arXiv:1912.08379.*
2. Oosterbaan, K.; 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." *chemrxiv.11328347.v1.*
3. 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.*
4. 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." *arXiv:1807.00821.*
5. Tubman, N.M. *et.al.* "Postponing the orthogonality catastrophe: efficient state preparation for electronic structure simulations on quantum devices." *arXiv:1809.05523.*
6. Levine, D.S.; **Hait, D**.; Tubman, N.M.; Whaley, K.B.; Head-Gordon, M. "ASCI-SCF analytic nuclear gradients and their application for geometry optimization of Ferrodoxin." *In preparation.*

Oral Presentations

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**.; Tubman, N.M.; Levine, D.S.; Head-Gordon, M. "Deterministic quantum chemistry of the uniform electron gas: An adaptive sampling configuration interaction (ASCI) approach." COMP Symposium on Quantum Mechanics. **ACS Boston 2018**.
4. **Hait, D**.; Head-Gordon, M. "Characterizing density and delocalization errors in DFT ." COMP Symposium on Recent Advances in DFT & TDDFT. **ACS Boston 2018**.
5. **Hait, D**.; Mavros, M.; Van Voorhis, T. "Condensed phase non-adiabatic dynamics from temporally-interpolated memory kernels." PHYS Symposium on Quantum Dynamics in Large Scale Systems. **ACS San Francisco 2017**.

Poster Presentations

1. **Hait, D**.; Rettig, A.; Head-Gordon, M. "Development of excited state quantum chemistry methods capable of describing photodissociation of single bonds." COMP Poster Session & Scimix. **ACS San Diego 2019**.
2. **Hait, D**.; Head-Gordon, M. "How Accurate is Density Functional Theory at Predicting Dipole Moments? **West Coast Theoretical Chemistry Symposium**, Stanford CA. March 2018.

3. **Hait, D**.; Mavros, M.; Van Voorhis, T. "Modeling Condensed Phase Electron Transfer Dynamics with Spin-Boson like Hamiltonians." PHYS Poster Session. **ACS Boston 2015**.

Teaching Experience

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).

Honors and Awards

CCG Graduate Research Excellence Award: Awarded by ACS COMP Division. 2019
Berkeley Fellowship: For graduate studies at UC Berkeley. 2016–2018
James R. Killian, Jr. (1926) Scholarship: For undergraduate studies at MIT. 2012–2016
Phi Beta Kappa Honor Society: Elected to the Xi Chapter (Massachusetts). 2016
Alpha Chi Sigma Award: Awarded by the MIT Chemistry department for outstanding achievement in scholarship, research, and service to the department. 2016
F.D. Greene Teaching Award: Awarded by the MIT Chemistry department. 2016
Sigma Pi Sigma Physics Honor Society: Elected to the MIT Chapter. 2016
Sophomore Achievement Award: Awarded by the MIT Chemistry department. 2014
Freshman Achievement Award: Awarded by the MIT Chemistry department. 2013
MIT-Sabanci Freshman Scholar: Selected for a one week exchange program to Sabanci University, Istanbul; based on academic performance in freshman year. 2013
International Chemistry Olympiad: Gold medalist (2011, 2012), Silver medalist (2010).
International Junior Science Olympiad: Silver medalist (2008).

Workshops

Telluride School of Theoretical Chemistry: One of 28 selected to attend. 2017
ACS PHYS Symposium Workshop for Undergraduate Chemistry Majors: One of 25 selected to attend. 2015

Activities

Peer Reviewer: *Molecular Physics.*
Chemistry Graduate Student Life Committee (UC Berkeley): Member (2016–present).
MIT Undergraduate Chemistry Association: Member (2014–2016), Co-president (2015-2016).