Diptarka Hait

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Research Interests
Theoretical and computational chemistry: Electronic structure theory, Nonadiabatic dynamics, Electronic excited states, Catalysis, Computational spectroscopy.

Experience

Stanford Science Fellow. Stanford University. Jul 2022–Current
Host: Professor Todd Martínez.

- Simulating the photochemistry and pump-probe spectra of organic molecules like cyclobutanone.
- Developing and applying GPU-accelerated methods for transition metal catalysis and periodic systems.
- Investigating excited state relaxation pathways of organic radical ions in collaboration with the Nocera group, for photoelectrocatalysis applications *(in preparation)*.
- Studying the role of nuclear quantum effects and nuclear dynamics in X-ray spectroscopies.
- Developed software for nonadiabatic dynamics with coupled cluster singles and doubles.

Education

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

- Developed an efficient and robust algorithm for excited state orbital optimization, and utilized it to accurately simulate time-resolved X-ray absorption (in collaboration with experimental spectroscopists).
- Described a new approach to study bond dissociation using static polarizability.
- Actively researched and published in other areas like selected configuration interaction, electrical response properties, catalysis, relativistic quantum chemistry, quantum computing, combustion, and corrosion.

S.B. in Chemistry and Physics. Massachusetts Institute of Technology. Sept 2012–Jun 2016
Research Advisor: Professor Troy Van Voorhis.
Thesis: Theoretical Studies on the Properties and Dynamics of Electronic Excited States. GPA: 5.0/5.0.

Awards

Stanford Science Fellow: Postdoctoral fellowship. 2022-2025
Young Investigator Award: ACS Division of Physical Chemistry. 2023
Nick Besley Award: For excellence in computational spectroscopy (Q-Chem corporation). 2023
Pimentel Research Award: To the most outstanding physical chemistry PhD (UC Berkeley). 2022
IBM-Zerner Graduate Student Award: 61st Sanibel Symposium. 2022
Finalist for Graduate Award in Theoretical Chemistry. ACS Division of Physical Chemistry. 2021
Finalist for Reaxys PhD Prize. 2020
CCG Graduate Research Excellence Award: ACS Division of Computers in Chemistry. 2019
Berkeley Fellowship: UC Berkeley (for graduate studies). 2016–2018
James R. Killian, Jr. (1926) Scholarship: MIT (for undergraduate studies). 2012–2016
Alpha Chi Sigma Award: For outstanding scholarship, research, and service (MIT Chemistry). 2016
F.D. Greene Teaching Award: MIT Chemistry. 2016
International Chemistry Olympiad: Gold medalist (2011, 2012), Silver medalist (2010).

Publications

44 publications in *Science*, *Angew. Chem.*, *Chem. Sci.*, *J. Phys. Chem. Lett.*, *J. Chem. Phys.*, *J. Chem. Theory Comput.*, *ACS Catalysis*, *PRX Quantum* etc.

(* indicates authors contributed equally)

44. Wang, Y; **Hait, D.**; Johnson, K.G.; Fajen, O.J.; Guerrero, R.D.; Martínez, T.J. "Extending GPU-Accelerated Gaussian Integrals in the TeraChem Software Package to f Type Orbitals: Implementation and Applications." *J. Chem. Phys.* **Accepted.** 244101. 2024. Preprint at *arXiv:2406.14920*.

43. Ou, J.H.; **Hait, D.**; Rupprecht, P.; Beetar, J. E.; Martínez, T.J.; Leone, S.R. "Attosecond Probing of Coherent Vibrational Dynamics in CBr_4." *J. Phys. Chem. A.* **ASAP**. 2024.

42. Ross, A.D.*; **Hait, D.***; Scutelnic, V.; Neumark, D.M.; Head-Gordon, M.; Leone, S.R. "Measurement of Coherent Vibrational Dynamics with X-ray Transient Absorption Spectroscopy Simultaneously at the Carbon K- and Chlorine $L_{2,3}$- Edges." *Commun. Phys.* **7,** 304. 2024.

41. **Hait, D.***; Lahana, D.*; Fajen, O.J.*; Paz, A.S.P.; Unzueta, P.A.; Rana, B.; Lu, L.; Wang, Y.; Kjønstad, E.F.; Koch, H.; Martínez, T.J. "Prediction of Photodynamics of 200 nm Excited Cyclobutanone with Linear Response Electronic Structure and Ab Initio Multiple Spawning." *J. Chem. Phys.* **160,** 244101. 2024.

40. Kang, R.; Zhao, Y; **Hait, D.**; Gauthier, J.A.; Kempler, P.A.; Thurman, K.A.; Boettcher, S.W.; Head-Gordon, M. "Understanding Ion-transfer Reactions in Silver Corrosion and Electrodeposition from First-principles Calculations and Experiments." *Chem. Sci.* **15**, 4996-5008. 2024.

39. **Hait, D.**; Martínez, T.J. "Predicting the X-ray Absorbtion Spectrum of Ozone with Single Configuration State Functions." *J. Chem. Theory Comput.* **20**, 873–881. 2024.

38. **Hait, D.**; Head-Gordon, M. "When Is a Bond Broken? The Polarizability Perspective." *Angew. Chem. Int. Ed.* **62**, e202312078. 2023. *Selected as a HOT Paper.* A **profile of D.H.** also appeared in the journal.

37. Toulson, B.W.*; **Hait, D.***; Faccialà, D.; Neumark, D.M.; Leone, S.R.; Head-Gordon, M.; Gessner, O. "Probing C-I Bond Fission in the UV Photochemistry of 2-Iodothiophene with Core-to-Valence Transient Absorption Spectroscopy." *J. Chem. Phys.* **159,** 034304. 2023.

36. 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." *Phys. Rev. X Quantum.* **4,** 030307. 2023.

35. Ridente, E.*; **Hait, D.***; Haugen, E.A.; Ross, A.D.; Neumark, D.M.; Head-Gordon, M.; Leone, S.R. "Femtosecond symmetry breaking and coherent relaxation of methane cations via x-ray spectroscopy." *Science.* **380**, 713-717. 2023.

34. Haugen, E.A.; **Hait, D.**; Scutelnic, V.; Xue, T.; Head-Gordon, M.; Leone, S.R. "Ultrafast X-ray Spectroscopy of Intersystem Crossing in Hexafluoroacetylacetone: Chromophore Photophysics and Spectral Changes in the Face of Electron Withdrawing Groups." *J. Phys. Chem. A.* **127**, 634–644. 2023.

33. 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.

32. **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.

31. Liang, J.; Feng, X.; **Hait, D.**; Head-Gordon, M. "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.* **18**, 3460-3473. 2022.

30. Klymko, K.; Mejuto-Zaera, C.; Cotton, S.J.; Wudarski, F.; Urbanek, M.; **Hait, D.**; Head-Gordon, M.; Whaley, K.B.; Moussa, J.; Wiebe, N.; de Jong, W.A. "Real time evolution for ultracompact Hamiltonian eigenstates on quantum hardware." *Phys. Rev. X Quantum.* **3**, 020323. 2022. **156,** 201104. 2022.

29. 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.

28. 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. (**D.H.** classified as mid-tier contributor out of three tiers).

27. Cunha, L.A.; Lee, J.; **Hait, D.**; McCurdy, C. W.; Head-Gordon, M. "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.

26. Shee, J.; Loipersberger, M.; **Hait, D.**; Lee, J. ; Head-Gordon, M. "Revealing the Nature of Electron Correlation in Transition Metal Complexes with Symmetry-Breaking and Chemical Intuition." *J. Chem. Phys.* **154**, 194109. 2021.

25. 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.

24. **Hait, D.**; Head-Gordon, M. "Orbital Optimized Density Functional Theory for Electronic Excited States." *J. Phys. Chem. Lett.* **12**, 4517-4529. 2021.

23. **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.

22. Yoneda, Y.; Mora, S.J.; 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.; Flemming, G.R.; "Electron-nuclear dynamics accompanying proton-coupled electron transfer." *J. Am. Chem. Soc.* **143**, 3104-3112. 2021.

21. 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.

20. Eriksen, J.J. *et al.* "The Ground State Electronic Energy of Benzene." *J. Phys. Chem. Lett.* **11**, 8922-8929. 2020. (Publication reporting results of a blind test, **D.H.** led the Berkeley team).

19. **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.
18. 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.
17. 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**, 8182-8192. 2020.
16. 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**, 2139-2159. 2020.
15. 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.
14. **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.
13. **Hait, D.**; Head-Gordon, M. "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." *J. Phys. Chem. Lett.* **11**, 775-786. 2020.
12. **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.*
11. **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.
10. 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.
9. **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.*
8. **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.
7. 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**, 5135-5142. 2018.
6. **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.*
5. **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.*
4. **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.
3. **Hait, D.**; Mavros, M.; Van Voorhis, T. "A hybrid memory kernel approach for condensed phase non-adiabatic dynamics." *J. Chem. Phys.* **147**, 014108. 2017.
2. Mavros, M.; **Hait, D.**; Van Voorhis, T. "Condensed phase electron transfer beyond the Condon approximation." *J. Chem. Phys.* **145**, 214105. 2016.
1. **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.

Selected Talks

- "Simulating nuclear quantum effects in X-ray absorption spectroscopy". PHYS Symposium on Energy Applications of Ultrafast Science. **ACS Denver, August 2024**.
- "Can excited states of radical ions act as photoredox catalysts?". **West Coast Theoretical Chemistry (WCTC), May 2024**.
- **Panelist for session on** "Soft X-ray Multipulse Multicolor Nonlinear Experiments in Solution - Experimental and Theoretical Opportunities". SSRL/LCLS Users' Meeting. **SLAC National Accelerator Laboratory, September 2023**. *(Invited)*.
- "Investigating the dynamics of Jahn-Teller distortion in CH_4^+ with time-resolved X-ray absorption". **Virtual International Seminar on Theoretical Advancements (VISTA), September 2023**.
- "Nonradiative relaxation mechanisms for electronic excited states of radical ions." PHYS Symposium in Honor of Marsha I. Lester. **ACS San Francisco, August 2023**.
- "Orbital optimized density functional theory for electronic excited states: Theory and Applications". Future Faculty Conference. **University of Chicago, June 2023**.
- "OO-DFT for Core-level Excitations and Applications to Molecular Symmetry Breaking". Besley Award Webinar. **Q-Chem, May 2023**. *(Invited)*.
- "Accurate prediction of core-level spectra from orbital optimized density functional theory: Theory and Applications". Photon Science Seminar. **SLAC National Accelerator Laboratory, October 2022**. *(Invited)*.
- "Orbital optimized density functional theory for core-level spectroscopy." PHYS Symposium in Honor of Prof. John F. Stanton. **ACS San Diego, March 2022**.
- "Orbital optimized density functional theory for electronic excited states" The Physical, Theoretical and Computational Chemistry Seminar. **Chemical Institute of Canada, October 2021**.
- "Orbital Optimized Density Functional Theory for Electronic Excited States". Pitzer Center Seminar for Theoretical Chemistry. **UC Berkeley, April 2021**.
- "Cheap and reliable optimization of excited state orbitals with the Square Gradient Minimization (SGM) approach." Division of Chemical Physics. **APS, March 2021**.
- "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, August 2019**.
- "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, August 2019**.

Teaching

- **Stanford:** Guest lecturer for Chem 261 (Computational chemistry: graduate level).
- **Berkeley:** Graduate Student Instructor for Chem 295 (Computational Quantum Chemistry: graduate level), Chem 120B (Physical Chemistry II), Chem 4A (General Chemistry for chemistry majors).
- **MIT:** Teaching Assistant for 10.637 (Quantum Chemical Simulations: graduate level), 5.61 (Physical Chemistry I).

Mentorship

Graduate Students:
Berkeley: Adam Rettig, Juan Arias-Martinez, Richard Kang, Leonardo dos Anjos Cunha, Hengyuan Shen.
Stanford: Yuanheng Wang, Ethan Curtis, Mingning Zhu, Dean Lahana, Garrett Kukier, Ruiyan Wang.
Undergraduate Students: Yu Hsuan Liang (Berkeley), Meaghan Pearson (Foothill College), Anna Robledo (Foothill College).
Subgroups: Leader of the excited state dynamics subgroup in the Martínez group.

Professional Activities

Peer Reviewer: *Proc. Natl. Acad. Sci. U.S.A.; 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).