Chenru Duan

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website(link)

EDUCATION

2017 – 2022 (expected) **Ph.D. in Chemistry, MIT**, Cambridge, MA, USA
Doctoral advisor: Prof. Heather J. Kulik, GPA: 4.8/5.0

2013-2017 **B.S. in Physics, Chu Kochen Honors College, Zhejiang University**, Hangzhou, China
Honored degree, GPA: 3.92/4.00 (Overall), 3.95/4.00 (Major)

RESEARCH EXPERIENCE

Nov. 2017 – Present **Department of Chemistry, MIT**, Cambridge, MA, USA
Graduate Research Assistant; Advisor: Prof. Heather J. Kulik

- Transformed quantum chemistry calculations with machine learning to achieve autonomous workflow for computational high throughput screening with higher efficacy and data quality
- Developed tools of multi-scale modeling using transfer learning and uncertainty quantification for simulating open-shell transition metal complexes
- Discovered functional materials by combining multi-objective optimization, virtual high throughput screening, and machine learning, such as redox couples in redox flow battery, single-site catalysts for methane-to-methanol conversion, and transition metal chromophores

July 2017 – Sept. 2017 **SMART Program, National University of Singapore**, Singapore
Research Engineer; Advisor: Prof. Jianshu Cao

- Uncovered novel heat transport behaviors in non-commutative quantum heat engine with heat-flux extended hierarchical equation of motion

July 2015 – June 2017 **Department of Physics, Zhejiang University**, Hangzhou, Zhejiang, China
Undergraduate Research Assistant; Advisor: Prof. Jianlan Wu

- Enabled numerical-exact calculations of open quantum dynamics *via* extending the domain of applicability of hierarchical equation of motion, and studied the quantum phase transition of the spin-boson model

HONORS AND AWARDS

2022 Excellence Award for Graduate Student, ACS Chemical Computing Group
MolSSI Software Fellow ($50,000 to support molecular science software development in MolSSI)

2021 Best Poster Award, International Symposium on Machine Learning in Quantum Chemistry
Gold Award, MRS Graduate Student Award
Graduate Student Award, AIChE's Computational Molecular Science and Engineering Forum

PUBLICATIONS

Total (up to Mar. 2022): 24 published, 1 in press, 3 submitted, 14 first-authored.
H-index: 14, Citations: 694 Google scholar page (link)

28. A. Nandy, **C. Duan**, C. Coffinet, and H. J. Kulik, "New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts", submitted (2022) (link)
27. **C. Duan**, A. Nandy, H. Adamji, Y. Roman-Leshkov, and H. J. Kulik, "Machine Learning Models Predict Calculation Outcomes with the Transferability Necessary for Computational Catalysis", submitted (2022) (link)
26. **C. Duan**, D. B. K. Chu, A. Nandy, and H. J. Kulik, "Detection of Multi-Reference Character Imbalances Enables a Transfer Learning Approach for Virtual High Throughput Screening with Coupled Cluster Accuracy at DFT Cost", submitted (2022) (link)
25. A. Nandy†, G. Terrones†, N. Arunachalam, **C. Duan**, D. W. Kastner, and H. J. Kulik, "MOFSimplify: Machine Learning Models with Extracted Stability Data of Three Thousand Metal–Organic Frameworks", *Sci. Data*, **9**, 74, (2022) (link)
24. **C. Duan**†, A. Nandy†, and H. J. Kulik, "Machine Learning for the Discovery, Design, and Engineering of Materials", *Annu. Rev. Chem. Biomol. Eng.* in press (2022)
23. M. Liu, A. Nazemi, M. G. Taylor, A. Nandy, **C. Duan**, A. H. Steeves, and H. J. Kulik, "Large-scale Screening Reveals Geometric Structure Matters More than Electronic Structure in Bioinspired Catalyst Design of Formate Dehydrogenase Mimics", *ACS Catal.,* **12**, 1, 383–396, (2021) (link)
22. A. Nandy†, **C. Duan**†, and H. J. Kulik, "Audacity of Huge: Overcoming Challenges of Data Scarcity and Data Quality for Machine Learning in Computational Materials Discovery", *Curr. Opin. Chem. Eng.*, **36**, 100778 (2021) (link)

21. A. Nandy, **C. Duan**, and H. J. Kulik, “Using Machine Learning and Data Mining to Leverage Community Knowledge for the Engineering of Stable Metal-Organic Frameworks”, *J. Am. Chem. Soc.*, **143**, 42, 17535–17547 (2021) (link)
20. **C. Duan**, S. Chen, M. G. Taylor, F. Liu, and H. J. Kulik, “Machine Learning to Tame Divergent Density Functional Approximations: A New Path to Consensus Materials Design Principles”, *Chem. Sci,* **12**, 39, 13021-13036 (2021) (link)
19. A. Nandy†, **C. Duan**†, M. G. Taylor, F. Liu, A. H. Steeves, and H. J. Kulik, “Computational Discovery of Transition-Metal Complexes: From High-throughput Screening to Machine Learning”, *Chem. Rev.* **121**, 16, 9927–10000 (2021) (link)
18. **C. Duan**, F. Liu, A. Nandy, and H. J. Kulik, “Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery”, *J. Phys. Chem. Lett.* **12**, 19, 4628–4637 (2021) (link)
17. J. P. Janet, **C. Duan**, A. Nandy, F. Liu, and H. J. Kulik, “Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design”, *Acc. Chem. Res.*, **54**, 3, 532–545 (2021) (link)
16. F. Liu, **C. Duan**, H. J. Kulik, “Rapid Detection of Strong Correlation with Machine Learning for Transition-Metal Complex High-Throughput Screening”, *J. Phys. Chem. Lett.*, **11**, 19, 8067–8076 (2020) (link)
15. **C. Duan**, F. Liu, A. Nandy, H. J. Kulik, “Semi-Supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost”, *J. Phys. Chem. Lett.* **11**, 16, 6640–6648 (2020) (link)
14. **C. Duan**, F. Liu, A. Nandy, H. J. Kulik, “Data-Driven Approaches Can Overcome the Cost–Accuracy Trade-off in Multireference Diagnostics”, *J. Chem. Theory Comput.* **16**, 7, 4373–4387 (2020) (link)
13. M. G. Taylor†, T. Yang†, S. Lin†, A. Nandy, J. P. Janet, **C. Duan**, and H. J. Kulik, “Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions”, *J. Phys. Chem. A* **124**, 16, 3286–3299 (2020) (link)
12. **C. Duan**, C.-Y. Hsieh, J. Liu, J. Wu and J. Cao, “Unusual Transport Properties with Non-Commutative System-Bath Coupling Operators”, *J. Phys. Chem. Lett.*, **11**, 10, 4080–4085 (2020) (link)
11. J. P. Janet, S. Ramesh, **C. Duan**, H. J. Kulik, “Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization”, *ACS Cent. Sci.*, **6**, 413–524 (2020) (link)
10. A. Nandy†, D. B. K. Chu†, D. R. Harper, **C. Duan**, N. Arunachalam, Y. Cytter, and H. J. Kulik, “Large-Scale Comparison of 3d and 4d Transition Metal Complexes Illuminates the Reduced Effect of Exchange on Second-Row Spin-State Energetics”, *Phys. Chem. Chem. Phys*. **22**, 19326-19341 (2020) (link)
9. A. Nandy, J. Zhou, J. P. Janet, **C. Duan**, R. B. Getman, and H. J. Kulik, “Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metal−Oxo Intermediate Formation”, *ACS Catal.* **9**, 9, 8243–8255 (2019) (link)
8. J. P. Janet, F. Liu, A. Nandy, **C. Duan**, T. Yang, S. Lin, and H. J. Kulik, “Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry”, *Inorg. Chem.* **58**, 16, 10592–10606 (2019) (link)
7. J. P. Janet, **C. Duan**, T. Yang, A. Nandy, and H. J. Kulik, “A Quantitative Uncertainty Metric Controls Error in Neural Network-Driven Chemical Discovery”, *Chem. Sci.* **10**, 7913-7922 (2019) (link)
6. **C. Duan,** J. P. Janet, F. Liu, A. Nandy, and H. J. Kulik, “Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models”, *J. Chem. Theory Comput.* **15**, 4, 2331–2345 (2019) (link)
5. C.-Y. Hsieh, J. Liu, **C. Duan**, and J. Cao, “A Nonequilibrium Variational Polaron Theory to Study Quantum Heat Transport”, *J. Phys. Chem. C* **123**, 28, 17196–17204 (2019) (link)
4. Q. Wang, Z. Gong, **C. Duan**, Z. Tang, and J. Wu, “Dynamical Scaling in the Ohmic Spin-Boson Model Studied by Extended Hierarchical Equations of Motion”, *J. Chem. Phys.* **150**, 084114 (2019) (link)
3. A. Nandy†, **C. Duan**†, J. P. Janet, S. Gugler, and H. J. Kulik, “Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry”, *Ind. Eng. Chem. Res*. **57**, 42, 13973–13986 (2018) (link)
2. **C. Duan**, Q. Wang, Z. Tang, and J. Wu, “The Study of an Extended Hierarchy Equation of Motion in the Spin-Boson Model: The Cutoff Function of the Sub-Ohmic Spectral Density”, *J. Chem. Phys.* **147**, 164112 (2017) (link)
1. **C. Duan**, Z. Tang, J. Cao, and J. Wu, “Zero-Temperature Localization in a Sub-Ohmic Spin-Boson Model Investigated by an Extended Hierarchy Equation of Motion”, *Phys. Rev.* B **95**, 214308 (2017) (link)
† These authors contribute equally.

ORAL PRESENTATIONS

8. Tencent Quantum Lab, “How Do Data-Driven Strategies Play a Role in Accelerating Quantum Chemistry Calculations for Inorganic Materials”, Dec. 2021, ***invited webinar***
7. Material Research Society (MRS), “Integrating Automated Quantum Chemistry Calculation Workflows with Machine Learning: Towards Faster Materials Discovery with Higher Fidelity”, Dec. 2021, Boston, MA, USA
6. American Institute of Chemical Engineers (AIChE) Annual Meeting, “Transforming Automated Quantum Chemistry Calculation Workflows with Machine Learning: Towards Faster Chemical Discovery with Higher Accuracy”, Nov. 2021, Boston, MA, USA
5. SIAM Conference on Mathematical Aspects on Materials Science, “How can Machine Learning Aid Computational Chemistry in Data Generation”, May 2021, ***invited talk***, virtual conference due to COVID-19 pandemic
4. Virtual American Institute of Chemical Engineers (AIChE) Annual Meeting, “A Database with Automated Quantum Chemistry Calculations and Machine Learning for Functional Transition Metal Complex Discovery”, Nov. 2020, virtual conference due to COVID-19 pandemic

3. TeraChem Developer Meeting, “Group Research Update: Inorganic Discovery in a Nutshell”, Sept. 2020, ***invited talk***, virtual meeting due to COVID-19 pandemic
2. New England Catalyst Society Winter Meeting, “Accelerating Catalyst Discovery by Predicting Electronic Structure Calculation Outcomes with a Machine Learning Decision Engine”, Jan. 2020, Worcester, MA, USA
1. American Physical Society (APS) March Meeting, **C. Duan,** J. P. Janet, F. Liu, A. Nandy and H. J. Kulik, “Accelerating Inorganic Discovery with Meta-Calculation Filtering *via* a Decision Classifier”, Mar. 2019, Boston, MA, USA

POSTER PRESENTATIONS

5. The International Symposium on Machine Learning in Quantum Chemistry (SMLQC), “Transforming Automated Quantum Chemistry Calculation Workflows with Machine Learning: Towards Faster and More Accurate Chemical Discovery”, Dec. 2021, virtual conference due to COVID-19 pandemic
4. Molecular Systems Design & Engineering (MSDE), “Transforming Automated Quantum Chemistry Calculation Workflows with Machine Learning: Towards Faster and More Accurate Chemical Discovery”, June 2021, virtual symposium
3. Virtual Conference on Theoretical Chemistry (VCTC), “Diagnosing Multireference Character with Machine Learning at Low Cost”, July, 2020, virtual conference due to COVID-19 pandemic
2. Material Research Society (MRS), “Accelerating Materials Discovery with Autonomous Job Control Systems Aided by Machine Learning”, Dec. 2019, Boston, MA, USA
1. American Chemical Society (ACS), “Accelerating Inorganic Discovery with Meta-Calculation Filtering *via* a Decision Classifier”, Aug. 2018, Boston, MA, USA

MENTORSHIP

2021	Adriana Ladera*, MIT Summer Research Program (University of South Florida, S.B. ’22. Now admitted to MIT Ph.D. Class of 2027)
	Julian Liu*, MIT Undergraduate Research Opportunities Program (MIT S.B. ’22)
2020	Gregory Schuette, MIT Department of Chemistry Peer Mentoring Program (Now graduate research assistant at Bin Zhang’s group at MIT)
	Shuxin Chen*, MIT Undergraduate Research Opportunities Program (MIT S.B. ’22. Now software engineer at Meta)
2019	Sahasrajit Ramesh*, Exchange Program for Master Thesis in Oxford (Now Senior Analyst, Aurora Energy Research, UK)

* indicates author on a published or in preparation manuscript with me

TEACHING AND SERVICE

Teaching Assistant for 10.637 Computational Chemistry; 5.111 Principles of Chemical Science; 5.60 Thermodynamics and Kinetics
Reviewer for IEEE Transactions on Neural Networks and Learning Systems, Computational Materials Science, *npj* Computational Materials, MRS Bulletin, Journal of Chemical Physics, Journal of Physical Chemistry Letter, and Israel Journal of Chemistry
Reporter for Material Research Society Fall Meeting, Boston, 2021
Poster Mentor for Women+ in Chemistry (WIC+) & Chemistry Alliance for Diversity and Inclusion (CADI) Poster Symposium, MIT, 2021
Member of Application Review Committee, MIT Summer Research Program (MSRP), MIT, 2022

SKILLS

Languages: native in Chinese, proficient in English
Programming Languages: proficient in Python, Bash, and MATLAB, intermediate in Fortran, C, and Mathematica
Machine Learning Packages: proficient in Pytorch, Tensorflow, and PyG, intermediate in Spektral
Quantum Chemistry: proficient in Terachem, Psi4, ORCA, and QChem
Working Efficiency: proficient in high performance computing, Jupyter, Plotly, Docker, and Colab

HOBBIES

Basketball and electronic games; Japaneses and Chinese anime; Hiking