

EDUCATION

Massachusetts Institute of Technology Chemistry, Chemical Engineering Advisor: Heather Kulik	Cambridge, USA 2017.09 -
Zhejiang University B.S in Physics, Honored Class	Hangzhou, China 2013.09 – 2017.07

RESEARCH EXPERIENCE

Zhejiang University (Hangzhou, China) Undergraduate Research Assistant	2015.07-2017.07
<ul style="list-style-type: none">• Open quantum system and its dynamics.• Method development for numerical calculation of quantum dynamics for model systems.	
Massachusetts Institute of Technology (Cambridge, USA) Exchange undergraduate student	2016.07-2016.11
<ul style="list-style-type: none">• Quantum phase transition of spin-boson model.	
Singapore-MIT Alliance Research and Technology (SMART) (Singapore) Research Engineer	2017.07-2017.09
<ul style="list-style-type: none">• Heat transport in novel quantum systems.	
Massachusetts Institute of Technology (Cambridge, USA) Graduate student	2017.11 -
<ul style="list-style-type: none">• Machine learning aided job control system for transition metal complex generation• Develop systematically-improvable computational tools for open-shell inorganic catalyst.	

PUBLICATION

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).
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)
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 (2018)
4. Q. Wang, Z. Gong, **C. Duan** and J. Wu, “Dynamical Scaling in the Ohmic Spin-Boson Model Studied by Extended Hierarchical Equations of Motion”, *J. Chem. Phys.* **150**, 084114 (2019).
5. **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 (2019)
6. J. P. Janet, F. Liu, A. Nandy, **C. Duan**, T. Yang, L. Sean 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 (2019)
7. 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 (2019)
8. A. Nandy, J. Zhu, 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.* ASAP (2019)
9. 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.* ASAP (2019)
10. **C. Duan**, C.-Y. Hsieh, J. Liu, J. Wu and J. Cao, “Unusual Transport Properties with Non-Commutative System-Bath Coupling Operators”, submitted (<https://arxiv.org/abs/1907.11262>).

*These authors contribute equally.