Hanggai Nuomin



EDUCATION

Duke University, U.S.A.

Ph.D. program in theoretical chemistry M.S. in ECE (machine learning track)

Wuhan University, China Bachelor of Science, Chemistry SEPTEMBER 2014 - JUNE 2018

September 2019 - Present

September 2022 - Present

RESEARCH EXPERIENCE

Ph.D. Student, Duke University

SEPTEMBER 2019 - PRESENT

- Identified quantum advantage zones in chemical dynamics and developed a universal scheme for ion trap quantum simulation of general dissipative chemical dynamics (experimentally verified), in collaboration with the Kim and Kenneth groups at Duke Quantum Center.
- Established a theoretical framework for multi-donor/multi-acceptor charge transfer, providing a clear perturbative description that extends beyond Fermi's golden rule. This framework is well-suited for characterizing coherent multiple charge transfers in molecular assemblies and has been implemented in the partial-summation package.
- Developed a dynamical polaron transformation quantum master equation which avoids the initial state problem of the traditional polaron transformation.
- Developed a new algorithm for simulating open quantum systems, improving tensornetwork computational efficiency by three orders of magnitude.
- Generalized the chain mapping technique in DMRG to the cases of multiple spectral densities
- Developed a method using non-unitary similarity transformations to modify the entanglement properties of evolving quantum systems.
- Developed a tensor-network software package (fishbone that contains basic infrastructures and the efficient methods that I developed for chemical dynamics simulations.

Research Assistant, University of Hong Kong (HKU) SEPTEMBER 2018 - JUNE 2019

- Constructed a full configuration interaction (FCI) solver for nuclei-electron non-Hermitian Hamiltonians.
- Explored many-body effects in crystal growth.

B.S. Thesis: Cooperativity in N-methylacetamide Backbones November 2017 - May 2018

- Received the nomination as an "outstanding undergraduate thesis."
- Analyzed the flaws of the definitions of cooperativity; proposed a correct definition of cooperativity with the advisor.
- Calculated the cooperativity of NMA chains using the new definition; found a scaling relation to predict the cooperativity in the absence of real quantum chemical calculations.

Honors Fellowship and Scholarship

- Duke Nanosciences Program Fellowship (2022)
- Marcus Hobbs Fellowship, Department of Chemistry at Duke University (2022)
- Wuhan University Scholarship for Excellent Students (2016, 2017)
- Wuhan University Scholarship for Excellent Freshman (2014)
- Scholarship for Students Majoring in Fundamental Sciences (2014)

Publications Book

1. D.N. Beratan, <u>H. Nuomin</u> et al., "Dynamical Quantum Chemistry: Hands-on Studies of Coherence in Chemistry", in preparation

Journal Articles

- 1. Z. Charyshnikova, <u>H. Nuomin</u>, & D.N. Beratan, "Influence of magnetic field on spin polarization in tight-binding models", in preparation
- 2. H. Halkhunaizi, J.D. Schultz, <u>H. Nuomin</u>, P. Zhang, & D.N. Beratan, "Prospects for enhancing triplet energy transfer using a tight-binding model Hamiltonian", in preparation
- 3. <u>H. Nuomin</u>, Z. Charyshnikova, N. Singh, K. Terai, P. Zhang, & D.N. Beratan "Theories of chirality induced spin selectivity: a pedagogical review", in preparation
- 4. <u>H. Nuomin</u>, P. Zhang, & D.N. Beratan, "Nonexponential length dependence of bridge-mediated electron transfer rates by breaking destructive interference", in preparation
- 5. <u>H. Nuomin</u>, P. Zhang, & D.N. Beratan, "Time-dependent polaron transformation", in preparation
- 6. G. Shwartz*, <u>H. Nuomin</u>*, D.N. Beratan, & J. Kim, "Quantum simulation of Hertzberg-Teller spectroscopy", in preparation
- 7. <u>H. Nuomin</u>, F.-F. Song, P. Zhang, & D.N. Beratan, "The properties of current induced chiral phonons recapitulate the characteristics of the CISS effect", in preparation
- 8. <u>H. Nuomin</u>, P. Zhang, & D.N. Beratan, "Condensed phase dynamics of multi-acceptor electron transfer", in preparation
- 9. F.-F. Song, <u>H. Nuomin</u>, & N. Kawashima, "Emergent intermediate phase in the J_1 - J_2 XY model from tensor network approaches", arXiv:2412.18892
- 10. K. Sun*, M.-Y. Kang*, <u>H. Nuomin</u>*, G. Schwartz, D.N. Beratan, K.R. Brown, & J. Kim, "Quantum simulation of spin-boson models with structured bath", arXiv:2405.14624
- 11. M.-Y. Kang, <u>H. Nuomin</u>, S.N. Chowdhury, J.L. Yuly, K. Sun, J. Whitlow, J. Valdiviezo, Z.-D. Zhang, P. Zhang, D.N. Beratan, & K.R. Brown, "Seeking a quantum advantage with trapped-ion quantum simulations of condensed-phase chemical dynamics", *Nat. Rev. Chem.* **8**, 340 (2024)
- 12. J.D. Schultz, J.L. Yuly, E.A. Arsenault, S.N. Chowdhury, R. Dani, S. Kundu, <u>H. Nuomin</u>, Z.-D. Zhang, J. Valdiviezo, P. Zhang, K.A. Parker, K. Orcutt, G.R. Fleming, N. Makri,

- J.P. Ogilvie, M.J. Therien, M.R. Wasielewski, & D.N. Beratan, "Coherence in chemistry: foundations and frontiers", *Chem. Rev.*, **124**, 11641 (2024)
- 13. <u>H. Nuomin</u>, J.-X. Wu, P. Zhang, & D.N. Beratan, "Efficient simulation of open quantum systems with multiple coupling channels to a reservoir", *J. Chem. Phys.* **161**, 124114 (2024)
- 14. <u>H. Nuomin</u>, F.-F. Song, P. Zhang, & D.N. Beratan, "Suppressing the entanglement growth in matrix product state evolution of quantum systems through nonunitary similarity transformations", *Phys. Rev. B* **106**(10), 104306 (2022)
- 15. <u>H. Nuomin</u>, D.N. Beratan, & P. Zhang, "Improving the efficiency of open-quantum-system simulations using matrix product states in the interaction picture", *Phys. Rev. A* **105**(3), 032406 (2022)
- 16. S. He, Y. Chen, M. Wang, <u>H. Nuomin</u>, P. Novello, X. Li & J. Liu, "Metal nitride nanosheets enable highly efficient electrochemical oxidation of ammonia", *Nano Energy*, **80**, 105528 (2021)

Published Abstracts

- 1. K. Sun, M. Kang, <u>H Nuomin</u>, K. Brown, J. Kim, & D.N. Beratan, Trapped-ion simulation of structured bath. *Bulletin of the American Physical Society* (2024).
- S. He, J. Liu, Y. Chen, M. Wang, <u>H. Nuomin</u>, & S. Zhu, "D-band contraction of metal nitride nanosheets enables highly efficient and stable electrochemical xxidation of ammonia", 239th ECS Meeting Abstracts, 40, 1297 (2021). The Electrochemical Society, Inc.

Service & Mentorship

Service

- Organized events and symposia for TriMolS, a community-driven initiative focused on molecular simulation in the Triangle region of North Carolina.

Mentorship

- Mentored an exchange student Jiaxi Wu in 2021-2022 at Duke, guiding him in complex open quantum system simulations using interaction-picture chain mapping. Jiaxi Wu was later admitted to Caltech's Physics Ph.D. program.

Skills Programming Languages and Development Tools

Python, C/C++, Julia, Mathematica, Vim, Bash, LTEX, TEX, HTML/CSS/JavaScript, Vue

Chemistry Software

ORCA, Gaussian, Q-Chem, SHARC

Quantum Software

QuTiP, Qiskit

Languages

English, Chinese (Mandarin), Mongolian