Hanggai Nuomin

nominhanggai.github.io
hanggai.nuomin@duke.edu

Education

Duke University, U.S.A.
Ph.D. program in theoretical chemistry — September 2019 - Present
M.S. in ECE (machine learning track) — September 2022 - Present

Wuhan University, China — September 2014 - June 2018
Bachelor of Science, Chemistry

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 tensor-network 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, **H. Nuomin** et al., "Dynamical Quantum Chemistry: Hands-on Studies of Coherence in Chemistry", in preparation

Journal Articles

1. Z. Charyshnikova, **H. Nuomin**, & D.N. Beratan, "Influence of magnetic field on spin polarization in tight-binding models", in preparation
2. H. Halkhunaizi, J.D. Schultz, **H. Nuomin**, P. Zhang, & D.N. Beratan, "Prospects for enhancing triplet energy transfer using a tight-binding model Hamiltonian", in preparation
3. **H. Nuomin**, Z. Charyshnikova, N. Singh, K. Terai, P. Zhang, & D.N. Beratan "Theories of chirality induced spin selectivity: a pedagogical review", in preparation
4. **H. Nuomin**, P. Zhang, & D.N. Beratan, "Nonexponential length dependence of bridge-mediated electron transfer rates by breaking destructive interference", in preparation
5. **H. Nuomin**, P. Zhang, & D.N. Beratan, "Time-dependent polaron transformation", in preparation
6. G. Shwartz*, **H. Nuomin***, D.N. Beratan, & J. Kim, "Quantum simulation of Hertzberg-Teller spectroscopy", in preparation
7. **H. Nuomin**, 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. **H. Nuomin**, P. Zhang, & D.N. Beratan, "Condensed phase dynamics of multi-acceptor electron transfer", in preparation
9. F.-F. Song, **H. Nuomin**, & 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*, **H. Nuomin***, 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, **H. Nuomin**, 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, **H. Nuomin**, 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. **H. Nuomin**, 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. **H. Nuomin**, 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. **H. Nuomin**, 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, **H. Nuomin**, 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, **H. Nuomin,**, K. Brown, J. Kim, & D.N. Beratan, Trapped-ion simulation of structured bath. *Bulletin of the American Physical Society* (2024).
2. S. He, J. Liu, Y. Chen, M. Wang, **H. Nuomin**„ & 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, LaTeX, TeX, HTML/CSS/JavaScript, Vue

Chemistry Software

ORCA, Gaussian, Q-Chem, SHARC

Quantum Software

QuTiP, Qiskit

Languages

English, Chinese (Mandarin), Mongolian