Xiaohan Dan

Postdoctoral Associate in Chemistry, Yale University (Oct 2023 - present)
Advisor: Prof. Victor S. Batista

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Education

09/2018-09/2023 **Ph.D. in Theoretical and Computational Chemistry, Supervisor: Prof. Qiang Shi**
Institute of Chemistry, Chinese Academy of Sciences

09/2014-06/2018 **B.S. in Applied Chemistry**
Beijing University of Chemical Technology

Research Interests

- **Fermionic open quantum system dynamics**: Developing new tools from full quantum and approximate methods, to study the energy or charge transfer between molecules and metal/electrochemical interfaces.

Publications

1. **Xiaohan Dan** and Qiang Shi, *Theoretical study of nonadiabatic hydrogen atom scattering dynamics on metal surfaces using the hierarchical equations of motion method*, ***J. Chem. Phys.*** 159, 044101 (2023).

2. **Xiaohan Dan**, Meng Xu, J. T. Stockburger, J. Ankerhold, and Qiang Shi, *Efficient low temperature simulations for fermionic reservoirs with the hierarchical equations of motion method: Application to the Anderson impurity model*, ***Phys. Rev. B*** 107, 195429 (2023).

3. **Xiaohan Dan**, Meng Xu, Yaming Yan, and Qiang Shi, *Generalized master equation for charge transport in a molecular junction: Exact memory kernels and their high order expansion*, ***J. Chem. Phys.*** 156, 134114 (2022).

4. Yu-Qi Wang, **Xiao-Han Dan**, Zhen-Yu Yi, Xiang Wang, Ya-Chen Feng, Yue Feng, Dong Wang, and Li-Jun Wan, *Single-Molecule Study on the Catalytic Role of Co–O2 Binding in ORR by In Situ ECSTM*, ***J. Phys. Chem. C***, 127, 6, 2929–2935 (2023).

5. Yu-Qi Wang, **Xiao-Han Dan**, Xiang Wang, Zhen-Yu Yi, JiaJu Fu, Ya-Chen Feng, Jin-Song Hu, Dong Wang, and Li-Jun Wan, *Probing the Synergistic Effects of Mg^{2+} on CO_2 Reduction Reaction on CoPc by In Situ Electrochemical Scanning Tunneling Microscopy*, ***J. Am. Chem. Soc.***, 144, 43, 20126–20133 (2022).

Skills

Theoretical methods	HEOM (Hierarchical equations of motion), GME (Generalized master equation), Tensor network
Programming	Fortran, Python, C/C++, LaTeX
Languages	Chinese, English, Japanese

Awards

- 2023 Excellent Poster Awards-First Prize, The 18th National Conference on Chemical Dynamics

- 2022 Merit Student, Institute of Chemistry, Chinese Academy of Sciences
- 2020 First Prize, Dimension Cup, National College Mathematical Contest in Modeling
- 2016 2017 National Encouragement scholarship, Beijing University of Chemical Technology

Conference presentations

2023	"Development of the fermionic hierarchical equations of motion method: Application to nonadiabatic hydrogen atom scattering dynamics on metal surfaces" **Contributed talk,** The 18th National Conference on Chemical Dynamics, Aug 17-20, 2023	Dalian, China
2022	"*Electron transport dynamics through molecule junctions: Generalized master equation and hierarchical equations of motion approaches*", **Contributed talk,** ACS Fall 2022 Meeting, Virtual Graduate Students Symposium in Asia-Pacific Region on Computational Chemistry, Aug 21-25, 2022	Chicago, IL, U.S.A (Virtual)
2021	*"Generalized master equation for charge transport in a molecular junction: Exact memory kernels and their high order expansion"*, **Poster**, The 14th National Conference on Quantum Chemistry, Oct 9-12, 2021	Shanghai, China