

## CV of Xiaoyu Xie

### Education

- 09/2010-06/2014 B.Sc., Science, School of Chemistry and Chemical Engineering, Nanjing University, China
- 01/2017-12/2017 CSC joint PhD in Prof. Alessandro Troisi's group, University of Warwick, UK
- 02/2019-04/2019 Visiting academic in Prof. Ulrich Schollwöck's group, Ludwig-Maximilians-Universität München, Germany
- 09/2014-12/2019 PhD student supervised by Prof. Chungen Liu and Prof. Haibo Ma, School of Chemistry and Chemical Engineering, Nanjing University, China

### Employment

- 03/2020-08/2023 Post-doctoral research associate (Prof. Alessandro Troisi's group), Department of Chemistry, University of Liverpool, UK
- 02/2024-now Researcher, School of Chemistry and Chemical Engineering, Shandong University, China

### Selected awards

- 2016 China Scholarship Council (CSC) Scholarship, China
- 2020 Seal of Excellence of Horizon 2020's Marie Skłodowska-Curie actions
- 2021 Seal of Excellence of Horizon 2021's Marie Skłodowska-Curie actions

### Research interests

1. Electron structure and exciton-phonon structure of excitons in molecular aggregates.
2. Time-dependent density matrix renormalization group and other quantum dynamics approach.
3. Quantum chemistry applications for optoelectronic processes in organic materials.
4. Quantum dynamics approaches for attosecond electronic dynamics.

### Teaching experience

1. Computational Chemistry II - Molecular Simulation, Nanjing University, China, 2013-2014. (Computational part)
2. Computational Chemistry II - Molecular Simulation, Nanjing University, China, 2014-2015. (Computational part)
3. Statistical Thermodynamics, Nanjing University, China, 2018-2019. (As assistant)
4. Modern Quantum Chemistry (undergraduate), Shandong University, China, 2025-2026.
5. Modern Quantum Chemistry, Shandong University, China, 2025-2026.
6. Physical Chemistry Experiment, Shandong University, China, 2025-2026.

- [1]. Z. Wang, **X. Xie\***, H Ma\*. Theoretical Investigation of Singlet Fission Processes in Organic Photovoltaics, *WIREs Comput. Mol. Sci.* **2025**, 15, e70002.
- [2]. Y. Cheng, Z. Xie, **X. Xie\***, H. Ma\*. Efficient Simulation of Inhomogeneously Correlated Systems Using Block Interaction Product States. *J. Chem. Theory Comput.* **2024**, 20, 9977-9990.
- [3]. J. Sun, R. Ma, X. Yang, **X. Xie**, D. Jiang, Y. Meng, Y. Li, F. Cui, M. Xiao, K. Zhang, Y. Chen, X. Xia, M. Zhang, X. Du, L. Ye, H. Ma, K. Gao, F. Chen, G. Li, X. Hao, H. Yin. Insulator-donor Electron Wavefunction Coupling in Pseudo-bilayer Organic Solar Cells Achieving a Certificated Efficiency of 19.18%. *Nat. Sci. Rev.* **2024**, 12, nwae385.
- [4]. Y. Liu<sup>#</sup>, **X. Xie<sup>#</sup>**, Q. Wang<sup>#</sup>, D. Chen, D. Qiu, X. Yan, L. Guo, Q. Chen, X. Zhang, H. Ju. Lighting and Rapid Detection of the Coronavirus S Protein using Computationally Speculated Ligand and Its Application in SARS-CoV-2. *Sensor Actuat. B-Chem.* **2024**, 418, 136284.
- [5]. X. Wu\*, **X. Xie\***, A. Troisi\*. Calibration of Several First Excited State Properties for Organic Molecules through Systematic Comparison of TDDFT with Experimental Spectra. *J. Mater. Chem. C* **2024**, 12, 18886-18892.
- [6]. K. Wang, Y. Xu, **X. Xie\***, H. Ma\*. Theoretical Investigation of Distal Charge Separation in a Perylenediimide Trimer. *J. Chem. Phys.* **2024**, 160, 164303.
- [7]. Z. Wang, **X. Xie\***, H. Ma\*. Simultaneous Intra- and Intermolecular Singlet Fission in Bipentacene Macrocycle Aggregates. *J. Phys. Chem. Lett.* **2024**, 15, 3523–3530.
- [8]. C. Ding<sup>#</sup>, **X. Xie<sup>#</sup>**, L. Chen, A. Troisi. Intuitive and Efficient Approach to Determine the Band Structure of Covalent Organic Frameworks from Their Chemical Constituents. *J. Chem. Theory Comput.* **2024**, 20, 1252-1262.
- [9]. Y. Lei, **X. Xie\***, H. Ma\*, J. Ma\*. Vitality of Intralayer Vibration in hBN for Effective Long-Range Interlayer Hole Transfer across High Barriers in MoSe<sub>2</sub>/hBN/WSe<sub>2</sub> Heterostructures. *J. Phys. Chem. Lett.* **2023**, 14, 11190–11199.
- [10]. Ö. H. Omar, **X. Xie**, A. Troisi, D. Padula. Identification of Unknown Inverted Singlet-Triplet Cores by High-Throughput Virtual Screening. *J. Am. Chem. Soc.* **2023**, 145, 19790–19799.
- [11]. Z. Wang, X. Yang, H. Ma\*, **X. Xie\***. Optimizing Through-Space Interaction for Singlet Fission by Using Macrocylic Structures. *J. Mater. Chem. C*, **2023**, 11, 21.
- [12]. **X. Xie\***, A. Troisi\*. Identification via Virtual Screening of Emissive Molecules with a Small Exciton–Vibration Coupling for High Color Purity and Potential Large Exciton Delocalization. *J. Phys. Chem. Lett.* **2023**, 14, 4119-4126.
- [13]. **X. Xie**, Y. Yao, H. Ma. Time-Dependent Density Matrix Renormalization Group for Quantum Chemistry. **2022**, in C. Zhu (Ed.) *Time-Dependent Density Functional Theory* (pp. 321-360). New York, Jenny Stanford Publishing.
- [14]. L. Shi<sup>#</sup>, **X. Xie<sup>#</sup>**, A. Troisi. Rapid Calculation of Internal Conversion and Intersystem Crossing Rate for Organic Materials Discovery. *J. Chem. Phys.* **2022**, 157, 134106.
- [15]. Y. Xu, Z. Xie, **X. Xie**, U. Schollwöck, H. Ma. Stochastic Adaptive Single-Site Time-Dependent Variational Principle. *JACS Au*, **2022**, 2, 335-340.
- [16]. **X. Xie**, A. Troisi. Evaluating the Electronic Structure of Coexisting Excitonic and Multiexcitonic States in Periodic Systems: Significance for Singlet Fission. *J. Chem. Theory Comput.* **2022**, 18, 394.
- [17]. C. Li, Y. Lei, H. Li, M. Ni, D. Yang, **X. Xie**, Y. Wang, H. Ma, W. Xu, X. Xia. Suppressing Non-Radiative Relaxation through Single-Atom Metal Modification for Enhanced Fluorescence Efficiency in Molybdenum Disulfide Quantum Dots. *Angew. Chem. Int. Ed.* **2022**, 61, e202207300.
- [18]. Z. Wang<sup>#</sup>, H. Liu<sup>#</sup>, **X. Xie<sup>#</sup>**, C. Zhang, R Wang, L. Chen, Y. Xu, H. Ma, W. Fang, Y. Yao, H. Sang, X. Wang, X.

- Li, M. Xiao. Free-Triplet Generation with Improved Efficiency in Tetracene Oligomers through Spatially Separated Triplet Pair States. *Nat. Chem.* **2021**, 13, 559–567.
- [19]. X. Zhang, W. Chen, **X. Xie**, Y. Zhang, Z. Chao, H. Ma, Y. Liu, H. Ju. Energy Pumping by Surface Collectors on Upconversion Nanoparticles for Extended Transfer and Efficient Self-Evaluable Photodynamic Therapy. *CCS Chem.* **2021**, 3, 1510–1521.
- [20]. **X. Xie**, C. Zhang, H. Ma. Charge Transfer via Deep Hole in the J51/N2200 Blend. *J. Chem. Phys.* **2020**, 153, 054705.
- [21]. L. Xiao, Z. Wang, C. Zhang, **X. Xie**, H. Ma, Q. Peng, Z. An, X. Wang, Z. Shuai, M. Xiao. Long Persistent Luminescence Enabled by Dissociation of Triplet Intermediate States in an Organic Guest/Host System. *J. Phys. Chem. Lett.* **2020**, 11, 3582-3588.
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- [23]. W. Li, J. Zhou, S. Cai, Z. Yu, J. Zhang, N. Fang, T. Li, Y. Wu, T. Chen, **X. Xie**, H. Ma, K. Yan, N. Dai, X. Wu, H. Zhao, Z. Wang, D. He, L. Pan, Y. Shi, P. Wang, W. Chen, K. Nagashio, X. Duan, X. Wang. Integrating High-Quality dielectrics with One-Nanometer Equivalent Oxide Thickness on Two-Dimensional Electronic Devices. *Nat. Electron.* **2019**, 2, 563.
- [24]. X. Zhang<sup>#</sup>, W. Chen<sup>#</sup>, **X. Xie**<sup>#</sup>, Y. Li, D. Chen, Z. Chao, C. Liu, H. Ma, Y. Liu, H. Ju. Boosting Luminance Energy Transfer Efficiency in Upconversion Nanoparticles with an Energy Concentrated Zone. *Angew. Chem. Int. Ed.* **2019**, 58, 12117.
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- [30]. W. Wang, X. Sun, J. Qu, **X. Xie**, Z.-H. Qi, D. Hong, S. Jing, D. Zheng, Y. Tian, H. Ma, S. Yu, J. Ma. Aggregation-Induced Visible Light Absorption Makes Reactant 1,2-Diisocyanoarenes Acting as Photosensitizer in Double Radical Isocyanide Insertions. *Phys. Chem. Chem. Phys.* **2017**, 19, 31443.
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- [34]. **X. Xie**, H. Ma. Opposite Anisotropy Effects of Singlet and Triplet Exciton Diffusion in Tetracene Crystal. *ChemistryOpen*, **2016**, 5, 201.

Attendance of Conferences and Workshops

- [1]. Symposium on Computational Statistical Mechanics of Complex Systems, Guangzhou, China, 2023, 'Fast Model Construction and Properties Evaluation of Excitonic Processes in Organic Systems' (Invited talk)
- [2]. Seminar for Young Scholars on Electronic Structure Theory and Methods, Jinan, China, 2019, 'Application of the Time-Dependent Density Matrix Renormalization Group Methods for Realistic Chemical Systems' (Invited talk)
- [3]. Workshop on Computational Statistical Mechanics for Complex Systems, Nanjing, China, 2019, 'Time-dependent Density Matrix Renormalization Group Quantum Dynamics for Realistic Chemical Systems' (Poster)
- [4]. Gordon Research Conference - Hybrid Electronic and Photonic Materials and Phenomena, Hong Kong, China, 2018, 'Nonlocal electron-phonon coupling in prototypical molecular semiconductor' (Poster)
- [5]. The Chinese Chemical Society Congress, Hangzhou, China, 2018, 'Nonlocal electron-phonon coupling in prototypical molecular semiconductor' (Poster)