Xin Chang

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Education:

Postdoc researcher. Jan. 2024-current University of Texas at Austin, McKetta department of chemical engineering, Austin, TX

PhD. Sep. 2018 – Dec. 2023 Temple University, chemistry department, Philadelphia, PA

M. Sc. Sep. 2009 – Jun. 2012. Xiamen University, chemistry and chemical engineering department, Xiamen, China.

B. Sc. Sep. 2003 – Jun. 2008 NanKai University, chemistry department, Tianjin, China.

Research of interest

I am interested in electronic structure theory in chemistry, specifically, multi-reference wavefunction method, such as valence bond theory, CASSCF. The excitation state and its dynamics are also a field in current research, such as exciton with its electronic spectra in semi-conductors. I currently am applying expanded Frenkel exciton theory in absorption and emission spectra of copolymer chromophores. My future research will also cover quantum computing, including Hubbard model in quantum circuits design.

Working skills

Program coding with Fortran, Python and MATLAB. Document editing: Microsoft Word, LaTex

Publications:

1. Ying, F.; Chang, X.; Su, P.; Wu, W. VBEFP: A Valence Bond Approach That Incorporates Effective Fragment Potential Method. *J. Phys. Chem. A* **2012**, 116 (7), 1846–1853.
2. Chang, X.; Su, P.; Wu, W. Internal Rotation Barrier of the XH3YH3 (X, Y = C or Si) Molecules. An Energy Decomposition Analysis Study. *Chem. Phys. Lett.* **2014**, 610–611, 246–250.
3. Chang, X.; Chen, Z.; Su, P.; Wu, W. The CO Rotation in the Gaseous Glycine. An Energy Decomposition Analysis Study. *Chem. Phys. Lett.* **2015**, 640, 194–200.
4. Chang, X.; Zhang, Y.; Weng, X.; Su, P.; Wu, W.; Mo, Y. Red-Shifting versus Blue-Shifting Hydrogen Bonds: Perspective from Ab Initio Valence Bond Theory. *J. Phys. Chem. A* **2016**, 120 (17), 2749–2756.
5. Balooch Qarai, M.; Chang, X.; Spano, F. C. Vibronic Exciton Model for Low Bandgap Donor–Acceptor Polymers. *J. Chem. Phys.* **2020**, 153 (24), 244901.
6. Chang, X.; Balooch Qarai, M.; Spano, F. C. HJ-Aggregates of Donor–Acceptor–Donor Oligomers and Polymers. *J. Chem. Phys.* **2021**, 155 (3), 34905.
7. Chang, X.; Balooch Qarai, M.; Spano, F. C. Intermolecular Charge Transfer in H- and J-Aggregates of Donor–Acceptor–Donor Chromophores: The Curious Case of Bithiophene-DPP. J. Phys. Chem. C 2022, 126 (44), 18784–18795.