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Jia Shi

Experience

Dec 2022-until now	Dept. of Physics, University of Central Florida, Research Scholar (Supervisor: Dr. Talat S. Rahman)

Education

Sept 2019-Sept 2022	Dept. of Physics, University of Central Florida, Visiting Ph.D. Student (Supervisor: Dr. Talat S. Rahman)
Sept 2014-Sept 2022	Dept. of Physics, University of Science and Technology Beijing, Doctor of Physics (master-doctor continuous study) (Supervisor: Dr. Qiang Gu)
Sept 2009-Jun 2013	Dept. of Physics, Zhejiang Ocean University, Bachelor of Physics

Research Interests

I am interested in fundamental quantum mechanical problems in condensed matter physics, especially in quantum materials. I have plenty of experience in the calculations of electronic, vibrational, optical, magnetic, photocatalytic properties of surface and nanomaterials. My current research is focused on exploring unique quantum behaviors and physical features of quantum materials, and predict the nanostructure and functional performance of two-dimensional quantum materials. Besides, I pay attention to fundamental physical characters of superconductors, such as Cooper paring mechanism in high-temperature superconductors, which are explored using DFT plus post-process method. Understanding the properties of excitons and light response in two-dimensional transition metal dichalcogenides to ultrafast external field using TDDFT calculations is also one of the topics that I am focusing on.

Principal Research Topics

- Multi-scale modeling of chemical reaction and related phenomena at surface
- Understanding microscopic process of photocatalysis at surface and nanomaterials
- Theory and modeling of vibrational, optical and magnetic properties of nanomaterials
- Understanding the response of surface and nanostructures to ultrafast external field
- Exploring the Cooper paring mechanism in high-temperature superconductor using beyond density functional theory

Professional Skills

Based on my research experiences, I am capable of the following research skills:

- Software**:** VASP, Material studio, Origin, Quantum Espresso, ASE, BerkeleyGW, Python, Fortran
- In-depth knowledge of physics, materials, and experiences in *ab initio* calculations based on density functional theory (DFT), time-dependent density functional theory (TDDFT), and data analysis.
- Scientific reviewer for *ACS Photonics*

Publications

1. **Jia Shi**, Volodymyr Turkowski, Talat S. Rahman, Dark-exciton energy splitting in monolayer WSe2: Insights from time-dependent density functional theory, Phys. Rev. B **107**, 155431 (2023).
2. **Jia Shi**, Naseem Ud Din, Tao Jiang, Duy Le, Volodymyr Turkowski, Qiang Gu, Talat S. Rahman, Thickness dependence of superconductivity in FeSe films, Eur. Phys. J. Plus 138 (6), 1-11 (2023).
3. **Jia Shi**, Wenyu Zhang, Qiang Gu, Ab Initio calculation of surface-controlled photocatalysis in multiple-phase $BiVO_4$, J. Phys. Chem. C 126, 9541-9550 (2022).
4. **Jia Shi**, Wenyu Zhang, Qiang Gu, Investigation of W/Mo co-doping with multiple concentrations in photocatalyst $BiVO_4$ by first-principles calculations, Solid State Commun. 351, 174794 (2022).
5. **Jia Shi**, Lei Wang, Qiang Gu, First-principles study of the co-effect of carbon doping and oxygen vacancies in ZnO photocatalyst, Chin. Phys. B 30, 026301 (2021).
6. Tianhui Zhao, Zhi Tang, Xiaoli Zhao, Hua Zhang, Junyu Wang, Fengchang Wu, John P Giesy, **Jia Shi**, Efficient removal of both antimonite (Sb (III)) and antimonate (Sb (V)) from environmental water using titanate nanotubes and nanoparticles, Environ. Sci. Nano 6 (3), 834-850 (2019).

Conference Presentations

1. Presentation: “Ultrafast charge dynamics and optical response in bilayer WSe2: impact of excitons and electron-phonon interaction”, 2023 APS March Meeting, Las Vegas, NV, USA.
2. Presentation: “Ultrafast charge dynamics and optical response in bilayer WSe2: impact of excitons and electron-phonon interaction”, Nanoflorida, Orlando, FL, USA.
3. Presentation: “Bright and dark excitons in 1L WSe2: a time-dependent density-functional theory analysis”, 2022 APS March Meeting, Chicago, IL, USA.
4. Poster Presentation: “Bright and dark excitons in 1L WSe_2: a time-dependent density-functional theory analysis”, The 2022 Annual Symposium of the Florida Chapter of the AVS Science and Technology Society (2022 FLAVS), Orlando, FL, USA.
5. Presentation: “Thickness dependence of superconductivity in FeSe films”, 2020 APS March Meeting, Denver, CO, USA.
6. Poster Presentation: “Thickness dependence of superconductivity in FeSe films”, The 2020 Annual Symposium of the Florida Chapter of the AVS Science and Technology Society (2020 FLAVS), Orlando, FL, USA.

7. Poster Presentation: “First-principles theory of FeSe film”, International Conference on Strongly Correlated Electron Systems 2017 (SCES 2017), Prague, Czech.