Dianwei Hou

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Education and Experience

IBS Center for Molecular Spectroscopy and Dynamics, Korea University **02/2023 -**

Charles University **08/2017 - 09/2022**

Major in Modeling of Chemical Properties of Nano- and Biostructures
Doctor of Philosophy (October 2022)

University of Chinese Academy of Sciences **09/2014 - 07/2017**

Major in Physical Electronics
Master of Engineering (July 2017)

Shaanxi University of Science and Technology **09/2009 - 07/2013**

Major in Applied Chemistry
Bachelor of Engineering (July 2013)

Research Interests

Multiscale interface modeling, molecular dynamic, SFG spectra modeling, machine learning, global optimization and structure prediction, computational materials design, heterogeneous catalysis, sub-nanometer clusters, nonlinear optics.

Publications

1. Hou, D.; Heard, C. J., Migration of zeolite-encapsulated Pt and Au under reducing environments. *Catal. Sci. Technol.* **2022**, *12* (5), 1598-1609.
2. Ament, K.; Köwitsch, N.; Hou, D.; Götsch, T.; Kröhnert, J.; Heard, C. J.; Trunschke, A.; Lunkenbein, T.; Armbrüster, M.; Breu, J., Nanoparticles Supported on Sub-Nanometer Oxide Films: Scaling Model Systems to Bulk Materials. *Angew. Chem. Int. Ed.* **2021**, *60* (11), 5890-5897.
3. Hou, D.; Grajciar, L.; Nachtigall, P.; Heard, C. J., Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum. *ACS Catal.* **2020**, *10* (19), 11057-11068.
4. Hou, D.; Nissimagoudar, A. S.; Bian, Q.; Wu, K.; Pan, S.; Li, W.; Yang, Z., Prediction and Characterization of $NaGaS_2$, A High Thermal Conductivity Mid-Infrared Nonlinear Optical Material for High-Power Laser Frequency Conversion. *Inorg. Chem.* **2019**, *58* (1), 93-98.
5. Sun, Y.; Yang, Z.; Hou, D.; Pan, S., Theoretical investigation on the balance between large band gap and strong SHG response in BMO_4 (M = P and As) crystals. *RSC Adv.* **2017**, *7* (5), 2804-2809.
6. Shi, G.; Zhang, F.; Zhang, B.; Hou, D.; Chen, X.; Yang, Z.; Pan, S., $Na_2B_6O_9F_2$: A Fluoroborate with Short Cutoff Edge and Deep-Ultraviolet Birefringent Property Prepared by an Open High-Temperature Solution Method. *Inorg. Chem.* **2017**, *56* (1), 344-350.
7. Lu, J.; Shi, G.; Wu, H.; Wen, M.; Hou, D.; Yang, Z.; Zhang, F.; Pan, S., Experimental and ab initio studies of two UV nonlinear optical materials. *RSC Adv.* **2017**, *7* (33), 20259-20265.
8. Huang, J.; Su, X.; Hou, D.; Lei, B.; Yang, Z.; Pan, S., First-principles study lone-pair effects of Sb (III)-S

chromophore influence on SHG response in quaternary potassium containing silver antimony sulfides. *J. Solid State Chem.* **2017**, *249*, 215-220.

9. Hou, D.; Yang, Z.; Pan, S., Electronic, bond order, linear optical properties of series of alkali-metal P-O-P linkage borophosphates. *J. Alloys Compd.* **2017**, *706*, 589-595.
10. Zhen, N.; Wu, K.; Wang, Y.; Li, Q.; Gao, W.; Hou, D.; Yang, Z.; Jiang, H.; Dong, Y.; Pan, S., $BaCdSnS_4$ and $Ba_3CdSn_2S_8$: syntheses, structures, and non-linear optical and photoluminescence properties. *Dalton Trans.* **2016**, *45* (26), 10681-10688.
11. Mutailipu, M.; Li, Z.; Zhang, M.; Hou, D.; Yang, Z.; Zhang, B.; Wu, H.; Pan, S., The mechanism of large second harmonic generation enhancement activated by Zn^{2+} substitution. *Phys. Chem. Chem. Phys.* **2016**, *18* (48), 32931-32936.
12. Mutailipu, M.; Hou, D.; Zhang, M.; Yang, Z.; Pan, S., Manipulation of birefringence via substitution of Sr^{2+} by Pb^{2+} based on the structure model of $LiSr_{1-x}Pb_xBO_3$ ($0 \leqslant x \leqslant 0.5$). *New J. Chem.* **2016**, *40* (7), 6120-6126.
13. Hou, D.; Lei, B.-H.; Pan, S.; Zhang, B.; Yang, Z., Influence of original and simulated microscopic units on SHG response in semi-organic NLO materials. *RSC Adv.* **2016**, *6* (46), 39534-39540.
14. Yang, Z.; Huang, X.; Liu, Q.; Hou, D.; Zhang, B.; Huang, S.; Pan, S.; Yang, Y.; Zhang, M., Cation effect investigation on electronic structure, magnetic and optical properties of $Li_2Pb_2CuB_4O_{10}$. *Chem. Phys.* **2015**, *447*, 60-63.
15. Hou, D., Horbatenko, Y., Ringe, S., Cho, M., Spontaneous Water Intercalation in Graphene Supported on Hydrophilic Substrates. (submitted)

Google Scholar: https://scholar.google.com/citations?user=nX1z1W0AAAAJ&hl=en

Skills

Codes: VASP, CASTEP, Quantum ESPRESSO, WIEN2k, Gaussian, ASE, Yambo, USPEX, CALYPSO, CP2K, and MATLAB.

Programming language: Julia**,** Python**,** Shell scripting