Dianwei Hou

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Education

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

Major in Modeling of Chemical Properties of Nano- and Biostructures

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

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.**, Hermann J., Nachtigall P., Heard, C. J., Optical properties of zeolite encapsulated sub-nanometer silver: A theoretical investigation. (Preparing for submission)

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