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主要研究方向

材料基础科学问题的多尺度模拟：

1. 金属结构材料力学性能的第一性原理及分子动力学模拟与表征。
2. 氢能材料(金属氢化物，配位氢化物，共价有机骨架材料)储氢机制及性能改善机理的第一性原理研究。

主要学术成果

1. **Y. Song,** J. H. Dai, X. M. Liang, R. Yang, *Influence of Dopants Ti and Ni on Bonding Interactions and Dehydrogenation properties of Lithium Alanate*, Phys. Chem. Chem. Phys. (2010) **12**, 10942-10949.
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3. **Y. Song** and R. Yang, *Decomposition mechanism of magnesium amide $Mg(NH_2)_2$*, Int. J. Hydrogen Energy, (2009) **34**, 3778-3783.
4. **Y. Song,** J. H. Dai, C. G. Li, and R. Yang, *Influence of dopants Ti and Ni on dehydrogenation properties of $NaAlH_4$: Electronic structure mechanisms*, J. Phys. Chem. C (2009) **113**, 10215-10221.
5. **Y. Song**, W. C. Zhang, and R. Yang, *Stability and bonding mechanism of ternary (Mg, Fe, Ni)H_2 hydrides from first principles calculations*, Int. J. Hydrogen Energy, (2009) **34**, 1389-1398.
6. **Y. Song**, R. Singh and Z.X. Guo, *A First-Principles Study of the Electronic Structure and Stability of a Lithium Aluminium Hydride for Hydrogen Storage*, J. Phys. Chem. B, (2006) **110**, 6906-6910.
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11. C. X. Shang, M. Bououdina, **Y. Song** and Z.X. Guo**,** *Mechanical Alloying and Electronic Simulations of (MgH_2+M) Systems (M=Al,Ti,Fe,Ni,Cu and Nb) for H Storage*, Int. J. Hydrogen Energy, (2004) **29**, 73-80.
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13. Z.X. Guo**,** M. Bououdina, **Y. Song** and C. Shang, *Mechanical Alloying and Electronic Simulation of Mg-Based Hydrogen Absorbing Materials*, in Advanced Materials and Processing, eds. S. Hanada, Z. Zhong, S.W. Nam and R.N. Wright, JIM, 2001, pp.2917-2920.
14. Y. L. Hao, R. Yang, **Y. Song**, Y. Y. Cui, D. Li, and A. Niinomi, *Formation of point defects in TiAl and NiAl*, Intermetallics, (2004) **12**, 951-956.
15. Y. L. Hao, R.Yang, **Y. Song**, Y. Y. Cui, D. Li, and M. Niinomi, *Concentration of point defects and site occupancy behavior in ternary Ni*Al alloys, Mater. Sci. Eng. A (2004) **365**, 85-89
16. Y. L. Hao, R. Yang, Q. M. Hu, D. Li, **Y. Song**, and M. Niinomi, *Bonding characteristics of micro-alloyed B_2 NiAl in relation to site occupancies and phase stability*, Acta Mater. (2003) **51**, 5545-5554.
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