THERMODYNAMIC TUNING AND DATABASE ON NEW ENERGY MATERIALS

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New energy materials have attracted many researchers' attention. Hydrogen is regarded as one of the most promising alternatives to the energy crisis due to its high heating value, wide availability, and environmental compatibility. The primary technical components of the hydrogen energy system cover the production, supply, storage, conversion, and employment of hydrogen, among which the storage and conversion of hydrogen are consistently the keys to the effective utilization of hydrogen energy. Studies of economic, highly efficient, and safe hydrogen storage materials are of great importance in fuel cell-based vehicles. On the other hand, the application of phase change materials (PCMs) for solar thermal-energy storage has received considerable attention in recent years due to their high storage density.

In recent years, our research effort has been focused in developing hydrogen storage and PCMs based on micro/nano-technology, Li ion battery, fuel cells, hydrogen sensors, etc. The promising nanomaterials for hydrogen storage materials such as MH_x: M= Mg, La, Ni, etc., alanate, borohydride, and MOFs were conducted in our lab. Several composite PCMs with good performance have been synthesized through in-situ assembly, and their applications in thermal regulation of gypsum boards are presented.

The data-driven research paradigm-integrated high-throughput calculations, database, and machine learning is appealing to accelerate new material development. Recently, we will introduce our results on establishing a Materials Genome Initiative database and the property prediction based on machine learning for hydrogen-storage materials. Finally, we will summarize the thermodynamic regulation and database construction for hydrogen/heat energy storage and some other recent results in my group.

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