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COMPUTATIONAL MATERIALS DESIGN FOR ENERGY AND ENVIRONMENTAL APPLICATIONS

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The world's dependence on fossil fuels has led to the need for alternate sources of energy as supplies dwindle, as well as a growing need to remove harmful compounds from the air. Hydrogen energy and lithium-ion batteries are promising candidates for supplanting fossil fuels for automobile applications while novel adsorbents like metal-organic frameworks (MOFs) are promising materials for removing harmful gases. To date, the author's researches have been concerned with both aspects of the fossil fuel problem. Regarding hydrogen energy, his researches are focused on understanding the thermodynamics of metal hydride reactions for hydrogen storage applications. Specifically, the goal is to screen thermodynamically promising metal hydride reactions from a full database of metal hydride mixtures using first-principles calculations. The large-scale screening approach ultimately provides a number of promising single-step or multi-step metal hydride reactions. On the other hand, his research focus in the field of the lithium-ion batteries is on fundamentally understanding the thermodynamics and redox properties of promising electrode materials which would directly affect the battery capacity. The author's researches on MOFs are related to investigating promising MOFs for the removal and separation of harmful gases. Quantum mechanical methods are used to screen and assess functional groups that would be incorporated into MOF ligands to preferentially adsorb harmful gases under humid conditions. In conclusion, his research goal is to contribute to the community for the transition to environmentally friendly ecosystems.

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