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Phase Transition of Rare-earth Metal Hydrides under High Pressure[1]

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Hydrogen is the lightest and smallest element in the periodic table. Despite its most simple electronic structure, enormous complexity can arise when hydrogen participates in the formation of solids. High pressure perturbs the free energy sufficiently to push the system into unexplored regions of the energy landscape, thus providing an excellent platform for the investigation of novel physics in hydrides such as metal-insulator transition, superconductivity as well as stoichiometric change. In this talk, I will overview recent progress on hydrides research under pressure in both theoretical works and experiments. Theoretical predictions on atomic positions and stoichiometry in hydrides under high pressure play a critical role to determine crystal structures of experimentally observed novel compounds, especially due to tiny scattering length of hydrogen atoms in solids. In addition, predicted physical property such as metallization and superconductivity in hydrides can guide experiments and experimental observations provide inputs for refinement of calculations I will show examples to highlight the importance of integrated experiment-theory collaboration to study rare-earth hydride under high-pressure.

[1]Energy Frontier Research in Extreme Environments (EFREE) Center