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Computer Simulation of Hydrogen Storage Capacity in Hydrogen Storage Materials[1] MASAHIKO KATAGIRI, VASILEIOS TSEROLAS, SHIGEKI SAITO, YASUSHI TAKEUCHI, JUN NAKAMURA, National Institute for Materials Science, HIROSHI OGAWA, National Institute of Advanced Industrial Science and Technology — Metal hydrides are the most promising materials for hydrogen storage, especially the lightweight metal alloy hydrides. Getting high hydrogen uptake is a part of the problem. The recent developments in the field of fuel cells and more particularly hydrogen storage under solid form have underlined the usefulness of the Pressure-Composition-Temperature (PCT) curves. For the calculation of PCT of RNi5 (R = La, Pr, Nd, and Sm), we consider a simple model on the basis of statistical mechanics. In addition, Molecular Dynamics (MD) simulations and grand canonical Monte Carlo (MC) simulations are performed to predict PCT curves. Molecular dynamics is a powerful tool in calculating free energy, including the fluctuation effects. However, the problem in MD is the accuracy. Then the grand canonical MC is also used to check the accuracy. We also demonstrate the first principle calculations on RNi5 and V-based materials with zero-point vibration effect.

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