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Towards predictor based design of thermodynamic and kinetic properties of complex materials for hydrogen storage

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A calculational approach for the design of new complex materials for hydrogen storage with favorable thermodynamic stability and enhanced diffusion kinetics is presented. By combining density functional theory (DFT) calculations on stable crystal structures and local coordination models with database methods, we perform large-scale screening studies to determine a number of potential alloys/mixtures with favorable thermodynamic stabilities and identify simple descriptors for subsequent materials prediction. Predictors for the kinetic properties of the materials are derived from combining materials screening with path techniques and harmonic transition state theory (TST) to identify materials parameters, e.g. the hydrogen binding energy, which correlate with the macroscopic diffusion rates. These predictors are then used to design new alloy/mixture compositions and ratios to favor structures with optimal diffusion kinetics. We present results from binary and ternary alkali-transition metal borohydrides and Perovskite based hydrogen permeable membranes, as well as results from studies of binary and mixed metal ammines. Results from the modeling of pathways and rates of dynamical processes involved in the ab-/desorption mechanisms will also be presented and compared to quasi elastic neutron scattering data.