Ab initio guided materials designing to enable hydrogen economy

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Hydrogen is one of the potential candidates of sustainable energy. However, there are challenges to be met before realization of hydrogen as an energy source. Known bottlenecks are inefficient storage and hydrogen induced mechanical degradation of structural materials. We recently investigated the feasibility of hydrogen storage in 2D carbon and boron-based materials using Density functional Theory (DFT) and Ab-Initio Molecular Dynamics simulations. The obtained hydrogen binding energies, dissociation barriers and capacities indicate that these materials can be promising for efficient hydrogen storage.
To tackle the problem of hydrogen induced degradation of steels, we investigated the effectiveness of finely dispersed nano-carbides to limit the diffusible hydrogen content. Although hydrogen solubility in most carbides is low, the hydrogen-carbon vacancies interplay, local atomic environment and interface geometry can lead to increased hydrogen solubilities. In our DFT-based study, we consolidated the effect of aforementioned parameters by studying hydrogen trapping in various carbides of interest.