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Deliquescence of $NaBH_4$ computed from density functional theory PING LI, WISSAM AL-SAIDI, KARL JOHNSON, University of Pittsburgh — Complex hydrides are promising hydrogen storage materials and have received significant attention due to their high hydrogen-capacity. The hydrolysis reaction of $NaBH_4$ releases hydrogen with both fast kinetics and high extent of reaction under technical conditions by using steam deliquescence of NaBH4. This catalyst-free reaction has many advantages over traditional catalytic aqueous phase hydrolysis. The first step in the reaction is deliquescence, i.e. adsorption of water onto $NaBH_4$ surface and then formation of a liquid layer of a concentrated $NaBH_4$ solution, which is quickly followed by hydrogen generation. We have used periodic plane wave density functional theory to compute the energetics and dynamics of the initial stages of deliquescence on the (001) surface of $NaBH_4$. Comparison of results from standard generalized gradient approximation functionals with a dispersion-corrected density functional show that dispersion forces are important for adsorption. We used DFT molecular dynamics to assess the elementary steps in the deliquescence process.

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