Hydrogen/Deuterium Adsorption and Absorption Properties On and In Palladium Using a Combined Plane Wave and Localized Basis Set Method

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Abstract

Detailed information on the H/D isotope effects for adsorption on the surface and absorption in the bulk is important for understanding the nuclear quantum effect. To achieve this purpose, we developed a new theoretical approach, namely, the combined plane wave and localized basis set (CPLB) method. By using the multi-component quantum chemical method, which takes into account the quantum effect of proton or deuteron, with localized part in CPLB method, direct analysis of H/D isotope effect about adsorption and absorption is achieved. In this study, we performed a theoretical investigation of the H/D isotope effects for adsorption on a Pd(111) surface and absorption in bulk Pd. We clearly showed H/D isotope effect on geometry during adsorption and absorption. Our developed CPLB approach is a powerful tool for analyzing the quantum nature of H/D in surface, bulk, and inhomogeneous systems.

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