Density functional theory study on the dehydrogenation of 1,2-dimethyl cyclohexane and 2-methyl piperidine on Pd and Pt catalysts

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We previously discovered one of the promising liquid organic hydrogen carrier (LOHC) materials; 2-(N-Methylbenzyl)pyridine (MBP) [ChemSusChem 11 (2018) 661-665]. In this study, we elucidated the reaction mechanism of MBP dehydrogenation on Pd(111) and Pt(111), using the computational approach. Since MBP is too large to clearly describe at density functional theory (DFT) level, we studied the dehydrogenation reaction of 1,2-dimehyl cyclohexane (DCH) and 2-methyl piperidine (MPD), which are two fragments of the MBP. Dehydrogenation reaction energy profiles were established after the optimization of adsorption configuration, and then RDS in each reaction sequence was determined based on Brønsted-Evans-Polanyi (BEP) relation. The activation energies of each RDS were calculated to predict that the dehydrogenation reaction of MBP on Pd(111) would be better than that on Pt(111).