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Adsorption and decomposition of methanol on Ru-Pt/boron-doped graphene surface: A DFT study

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The decomposition reaction of methanol is currently attracting research attention due to the potential widespread applications of its end products. In this work, a periodic density functional theory (DFT) calculations have been performed to investigate the adsorption and decomposition of methanol on Ru–Pt/boron doped graphene surface. It was found that methanol (CH_3OH) decomposition through O-H bond breaking to form methoxide (CH_3O) as the initial step, followed by further dehydrogenation steps which generate, formaldehyde (CH_2O), formyl (CHO), and carbon monoxide (CO), is found to be the most favorable reaction pathway. The results showed that CH_3OH and CO groups prefer to adsorb at the Ru-top sites, while CH_2OH, CH_3O, CH_2O, CHO, and H_2 groups favor the Ru-Pt bridge sites, showing the preference of Ru atom to adsorb the active intermediates or species having lone-pair electrons. Based on the results, it was found that the energy barrier for CH_3OH decomposition through the initial O-H bond breaking is less than its desorption energy of 0.95eV, showing that CH_3OH prefers to undergo decomposition to CH_3O rather than direct desorption. The study provides in-depth theoretical insights into the potentially enhanced catalytic activity of Ru–Pt/boron doped graphene surface for methanol decomposition reactions, thereby contributing to the understanding and designing of efficient catalyst at optimum condition.

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