DFT Study of Methanol Decomposition on Ru-Pt clusters supported on Boron and Nitrogen Co-doped Graphene Surface

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Over the past few decades, there has been a great attention in finding alternative clean energy resources due to the decrease in fossil fuels. Among them, Hydrogen is considered as a clean and high efficient energy carrier because of its abundant availability and environmental friendliness. [1] At present, a number of different methods are used to produce the hydrogen. In addition, hydrogen production from renewable sources such as biomass and natural gas is also considered. Among the various natural gases, methanol has been regarded as an excellent H2-containing source because of its biodegradability. [2] The decomposition of methanol over metal catalyst has been suggested as an efficient way to generate hydrogen, however, the use of catalyst has some shortcomings such as poisoning of catalyst sites. Recently, graphene has been demonstrated as a very effective support for electro catalysts for methanol and hydrogen fuel cells due to its less CO poisoning. [3] To further improve the catalytic activity of graphene supported material, here we considered Boron-nitrogen co-doped graphene (BNG) support for Ru-Pt clusters and investigated the methanol decomposition using density functional theory calculations. The calculated adsorption energies for methanol on different possible sites of Ru-Pt / BNG surface are -0.61 eV to -0.99 eV, which are larger than methanol adsorbed on Pt(111) and Ru(001) surfaces. We considered two possible methanol decomposition pathways including dehydrogenation via the O-H bond breaking to form methoxide (CH3O) and the C-H bond breaking to form hydroxymethyl (CH2OH) as an initial steps. We also considered the dehydrogenation reactions from the initial steps for the hydrogen production. We found that the calculated reaction barriers for the methanol decomposition is significantly lower than the previous studies of pure and doped metal surfaces. Our results indicate that one-layer Ru-Pt clusters supported BNG surface is an economical catalyst for the hydrogen production via methanol decomposition compared to pure Pt surface.

References:

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