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Ab Initio Study of Atomic and Molecular Adsorption to Pt Clusters on Graphenes GYUBONG KIM, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — In recent years, Pt nanostructures have received a great deal of attention because of their exceptional chemical/electrochemical reaction properties with high catalytic efficiency. Particularly, a number of studies have focused on their versatile catalytic properties depending on their sizes, shapes, substrate and/or alloy compositions *etc.* Motivated by those studies, we investigated the adsorption of several important adsorbates (H, O, and CO) to Pt_x-graphene complexes (x = 1 or 13) with the use of *ab initio* density functional methods. Our calculations of Pt adsorption on various graphene defects demonstrate that Pt *d* band profiles remarkably vary depending on the type of graphene defects and the corresponding adsorption strength of the adsorbates is also substantially affected. Also for $Pt_{13}-$graphene complexes, the overall adsorption strength of H, O, and CO is remarkably changed depending on graphene defects, which indicates the variation of their catalytic behavior. The role of graphene defects for the interaction between Pt and the adsorbates will be presented.

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