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Theoretical Investigation of Gas Adsorption on Metal- Graphene Surface

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Abstract : Carbon nanostructures are of great importance in academic research and industry, which can be mentioned to chemical sensors, catalytic processes, pharmaceutical and environmental issues. Common point in all of these applications is the occurrence of adsorption of molecules on these structures. Important carbon nanostructures in this case are mainly nanotubes and graphene. To modify pure graphene, recently, many experimental and theoretical studies have carried out to investigate of metal adsorption on graphene. In this work, the adsorption of CO molecules on pure graphene and on metal adatom on graphene surface has been simulated based on density functional theory (DFT). All calculations were performed by PBE functional and Troullier-Martins pseudopotentials. Density of states (DOS) for graphene-CO, graphen and CO around the Fermi energy has been moved and very small mixing occured which implies the physisorption of CO on the bare graphen surface. While, the results have showed that CO adsorption on transition-metal adatom on graphene surface is chemisorption.

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