A density functional investigation of ethylene adsorption on graphene and VIIIB metal-doped graphene surfaces

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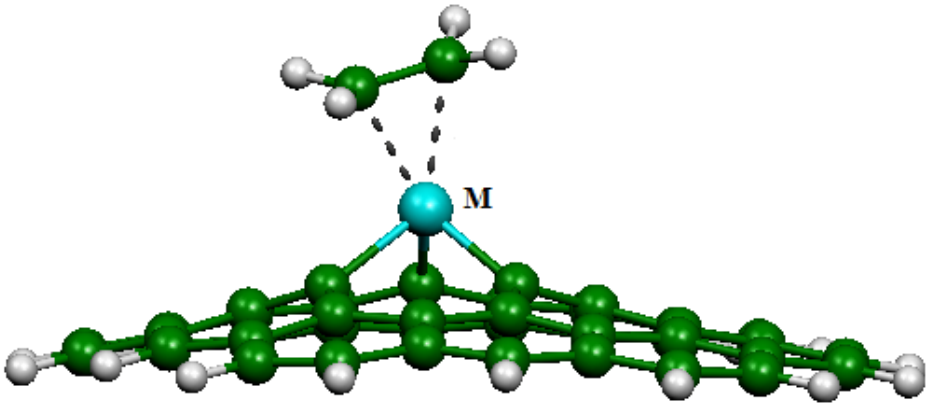
The ethylene adsorption on graphene and VIIIB metal-doped graphene (Fe-, Ru-, Os, Co-, Rh-, Pd-, Ir-, Ni- and Pt) sheets was investigated by means of density functional theory at the B3LY/LanL2DZ theoretical level. The graphene model composed of 14 benzene rings with the edge carbons terminated by hydrogen atoms ($C_{42}H_{48}$). For metal-doped graphene model, the carbon atom at the center of the sheet was replaced with metal atom ($MC_{41}H_{48}$). It is found that all metal-doped graphene sheets can adsorb ethylene molecule via exothermal process. Structural and energetic properties are also reported.



The configuration of ethylene adsorbed on metal–doped graphene sheet.