Graphene nanoribbon on Pt(111): Adsorption of oxygen atom and substrate interaction

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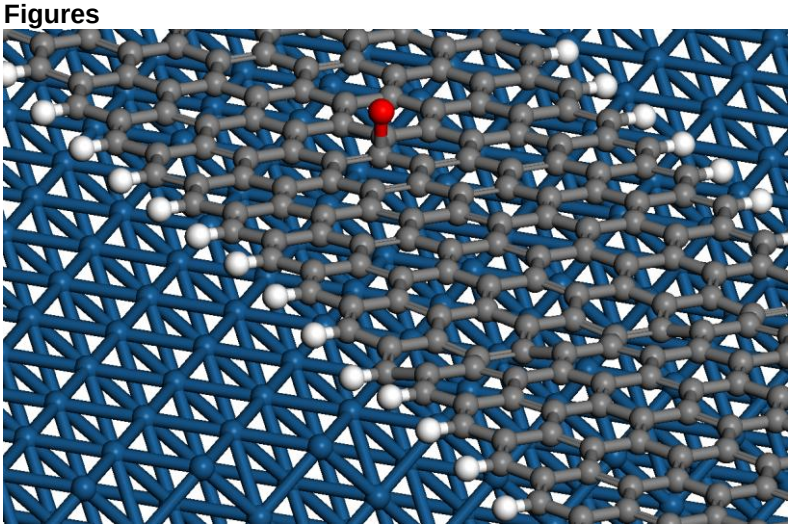
Abstract
Adsorption of oxygen atom on graphene nanoribbon(GNR)/Pt(111) surface has been studied using ab initio electronic structure calculations based on the density functional theory. The lattice mismatch between GNR and Pt(111) surface is considered here. We present the results of binding energy of oxygen atom on GNR/Pt(111) surface depending on adsorption sites and their corresponding electronic structures. These results are compared with those of oxygen adsorption on Pt(111) only. Also, we systematically examine the interaction between oxygen atom and strained GNR on Pt(111).

Figures



Oxygen adsorption on GNR/Pt(111) surface. Blue, gray, red, and white balls are platinum, carbon, oxygen and hydrogen atoms, respectively.