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**Binding of $N_2$, $O_2$, CO and $H_2O_2$ on graphene in the presence of Co** SHYAM KATTEL, BORIS KIEFER, Physics Department, New Mexico State University — One of the largest challenges in the current century is the production of energy to meet the increasing societal demands. Bio-inspired carbon based catalytic materials have been invoked as a possible solution to this challenge. We use density-functional-theory (DFT) to study molecule-Co-graphene interactions. Our results show that the most stable Co binding site is above the center of C6 hexagons of the graphene sheet (H) site in agreement with previous work. For molecule-Co-graphene interactions we find that $N_2$, $O_2$ and CO physiosorb onto the Co-graphene system only if the molecule and Co are on the same side of a graphene sheet. Therefore unaltered graphene is unlikely to be a catalytically active. In contrast we observe that $H_2O_2$ chemisorbs. These two different behaviors may explain selectivity of some catalytic materials toward $O_2$. We also observe that Co modifies the charge density only locally and which indicates that electronic transport properties of the underlying carbon structure are not enhanced and remain a bottleneck for the development of carbon based catalytic materials.

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