A First-principles study of CO oxidation on heteroatom-doped penta-graphene

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Abstract: We report a systematic study of CO oxidation over nitrogen- and boron-doped penta-graphene by using density functional theory (DFT) calculations. This work is to investigate the possibility of synergized O_2 activation by CO for CO oxidation on the substrate. CO oxidation takes place via the following processes: (i) $CO + O_2 \rightarrow OOCO \rightarrow CO_2 + O$ and $CO + O \rightarrow CO_2$ (ii) $2CO + O_2 \rightarrow CO_3 + CO \rightarrow 2CO_2$ and (iii) a new mechanism of $2CO + O_2 \rightarrow OCO - OCO \rightarrow 2CO_2$. Eley–Rideal (ER), Langmuir–Hinshelwood (LH) and tri-molecular Eley–Rideal (TER) mechanisms are proposed for the three processes. According to the small barriers of the rate-limiting steps for the ER, LH and TER mechanisms, these mechanisms are able to occur at low temperature. The current study may provide valuable clues for developing low-cost and higher catalytic carbon-based materials, and then open a new avenue for CO oxidations.

Keywords: CO oxidation, penta-graphene, reaction mechanism.

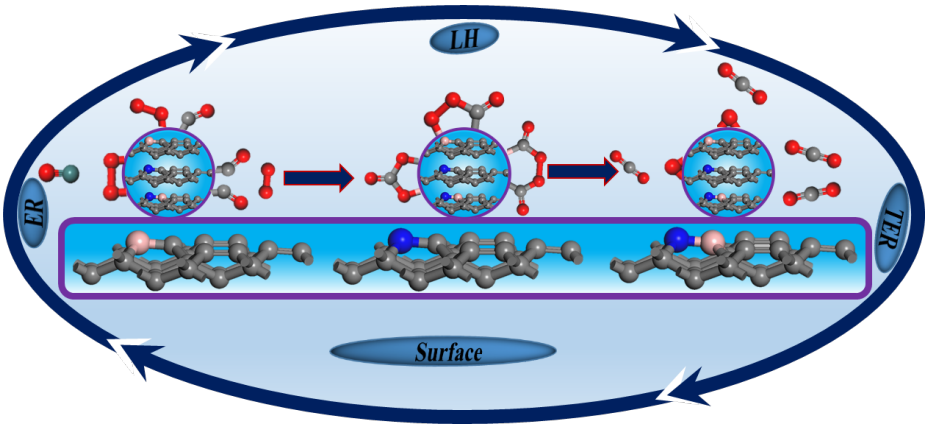

Figure 1. Reaction mechanisms for CO oxidation on the heteroatom-doped penta-graphene.

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