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Ab Initio Molecular Dynamics calculations on NO oxidation over oxygen functionalized High Oriented Pyrolytic Graphite.

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Nitrogen monoxide (NO) belongs to the group of the most polluting gases in the atmosphere. It serves as a critical precursor for the formation of smog and acid rain, which currently pose significant environmental and human health challenges. Carbonaceous materials have been identified as promising support to carry out the catalytic oxidation of NO to NO₂ at room temperature. After NO oxidation the NO₂ can be easily removed from the reaction chamber by the water scrubbing method allowing an efficient control of NO emissions. The understanding of the reaction mechanism involved in this complex process is fundamental to developing practical applications for this decontamination method.

We presented here ab initio molecular dynamics (AIMD) calculations on the NO oxidation over oxygen functionalized High Oriented Pyrolytic Graphite (O-HOPG) surface. Four different NO incidence energies were studied and the initial conditions were selected in order to facilitate the collision between the incident molecule and the epoxy group present at the surface. Our simulation results indicate that the reaction probability (HOPG-O + NO_(g) → HOPG + NO_{2(g)}) increase with the NO incidence energy. The correlations obtained between the initial molecule orientation and the reactivity shed light on the factors that facilitate the catalytic oxidation of NO over activated carbonaceous surfaces.