GRAPHENE REACTIONS WITH WATER AND CARBON DIOXIDE ON ARMCHAIR SITES

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In a previous study, we used density functional theory to analyze oxygen transfer reactions on graphene edges. This leads to interesting results and comparisons among the reactions of the following reactants: NO, O_2, H_2O and CO_2. However, the studies where narrowed to the analysis of zigzag sites only, and focused on carbene-like sites. Kinetic experimental results have reported specific energy barriers for desorption of products, indicating the presence of defined active sites or ready-to-desorb functional groups which are active at specific temperatures. To complete our analysis, it is required to extend our study to include other actives sites such as carbyne-like armchair sites. This ongoing work might explain some of the still unclear experimental facts, and make a difference on the reactivity of zigzag and armchair sites in the scope of the oxygen transfer reactions. Possible applications include theoretical and practical issues, such as the development of a quantification method of specific sites, new technologies for gasification or new materials.