A DFT analysis of the adsorption of nitrogen oxides on Fe-doped graphene, and the electric field induced desorption

Density functional theory calculations were carried out to study the adsorption and sensing properties of Fe-doped graphene nanosheets (FeG) toward nitrogen oxides (NO, NO2, and N2O). The results indicated the adsorption of nitrogen oxides is significantly increased onto FeG compared to pristine graphene, reaching adsorption energies of 1.1–2.2 eV, even with a high stability at room temperature. As a result of the larger charge transfer and strong chemical binding, the bandgap of the adsorbent-adsorbate systems is increased in up to 0.5 eV with respect to the free FeG, indicating that FeG is highly sensitive to nitrogen oxides. It was also evidenced the adsorption and sensing properties remain even in the presence of O2 currents for N2O, where a co-adsorption mechanism was analyzed. Besides, NO2 is capable to induce the largest magnetization of FeG. Finally, positive electric fields of at least 0.04 a.u. decrease the stability of the adsorbent-adsorbate interactions, inducing the desorption process. Therefore, FeG emerges as a promising low-dimensional material with excellent adsorption and sensing properties to be applied in solid state sensors of nitrogen oxides, where electric fields can be used as a strategy for the FeG reactivation in repetitive sensing applications.