Computational investigation of dispersion at the graphene interface

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Abstract: Thousands of mutagenic and carcinogenic chemicals are produced in tobacco smoke. To reduce health hazard risk of smoking patients, a cigarette filter tip containing cellulose acetate has been introduced by manufacturers. Carbon-based porous materials are promising adsorbents to enhance the removal efficiency of harmful compounds in cigarette mainstream smoke. This work focuses on computational modelling of tar, polycyclic aromatic hydrocarbons (PAHs) and organic toxicants, in comparison with nicotine, adsorbed on the graphene surface. Noncovalent interaction energetics of each complex were computed using dispersion-corrected density functional theory (DFT) methods. The results reveal that strong pi-pi interactions reflect the efficiency of adsorption. In addition, nitrogen-doped graphene shows stronger interaction than pristine graphene to the studied adsorbates. Graphene-based material could potentially be used as an adsorbent for the removal of some harmful organic compounds.

Keywords: Density functional theory; Polycyclic aromatic Hydrocarbons; Graphene; Nicotine; Interaction energy