Adsorption of Sarin on MgO Nanotubes: Role of Doped and Defect Sites

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Sarin (GB), isopropyl methylphosphonofluoridate ($C_4H_{10}FO_2P$), is a highly toxic organophosphorus chemical warfare agent which was developed for use in military operations. In this work, adsorption of sarin on the intrinsic and Ti-doped (doped at 3c and 4c site) MgO nanotube has been investigated. For this purpose, the structural and electronic characteristics of nanotubes are studied. The various characteristics of nanotubes, like binding energy, HOMO and LUMO energies, and average bond lengths are investigated and it is found that doping with Ti leads to modification in properties of the nanotube. Adsorption of sarin on intrinsic and doped nanotubes shows that adsorption proceeds through formation of covalent bonds between the molecule and the surface. These results are supported by changes in structural and electronic parameters of the molecule after adsorption. For all cases, adsorption is more favourable at low-coordinated sites, *i.e.* 3c site is preferred over 4c. Surface defects in MgO nanotubes arising from atom, ion, and MgO vacancies are also investigated. The adsorption of sarin at these defect sites of the MgO nanotube produces interesting products. The kind of defect in nanotube decides whether it will behave as an electron donor or as an acceptor.