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The properties of single-walled carbon nanotubes (SWCNTs) and their large specific surface area make these nanostructures potential materials for gas and energy storage. By accompanying such properties with the capability of being sensitive to the adsorbed molecules, SWCNTs would certainly appear as the ideal systems for different calculations and studies. Indeed, recent theoretical and experimental [1] reports claim that an exposure to ppm of molecules such as different kinds of gas adsorption can significantly affect the electronic and transport properties of the SWCNTs. The potential use of carbon nanotubes in H\textsubscript{2} storage is receiving considerable interest worldwide because materials that can store large amounts of hydrogen under practical conditions are desirable for emerging fuel-cell-powered vehicles at room temperature and moderate pressures have been reported for SWNTs [2]. The positive point of these results is that studies could be extended for other nanostructures such as silicon carbide nanotubes (SiCNTs). All the calculations have been carried out using Gaussian 03 software [3] and in vacuum. The Lennard-Jones potential energy system is a very simple system to get the optimum adsorption distance. It is defined by two independent parameters, σ and ε via the Lennard-Jones potential \( V(r) = 4\varepsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \).

So Lennard–Jones parameters in this study for SWCNPs are σ = 1.2 and ε = 736.74588 (Fig.1) and Lennard–Jones Parameters in this study for SWCNPs are σ = 1.4 and ε = 741.12 (Fig.2). The best adsorption sites for H\textsubscript{2} are the parallel approach of the molecule to the nano planar wall of a hexagon of silicon and carbon atoms in sites on SiCNT surfaces and the center of the carbon hexagonal for the parallel configuration in sites on CNT surfaces. This might have potential for gas detection and energy storage. The adsorption results in strong Si–H bindings and charge transfers from the H\textsubscript{2} molecule toward the SiC nanoplanar. The quantum MD simulation, carried out at room temperature, shows that the SiCNT/H\textsubscript{2} system is quite stable than CNT/H\textsubscript{2}. The rate of adsorption of H\textsubscript{2} by silicon carbide nanoplanar is faster than it by carbon nanoplanar. The theoretical results should be confirmed experimentally.

REFERENCES