Molecular dynamics of reactions between hydrogen peroxide and zigzag carbon nanotube.

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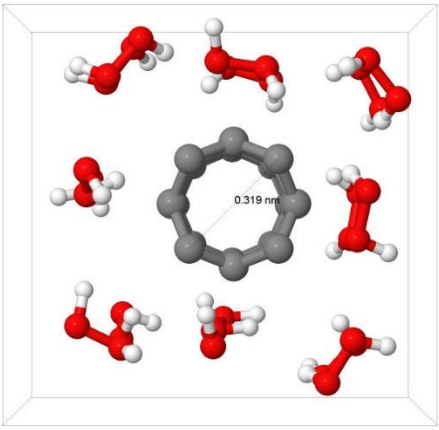
Single wall carbon nanotube (CNT) and graphene sheets have been suggested as a potential material for use in next generation gas sensors. Sidewall functionalization (impurities) onto CNTs help to facilitate gas molecule adsorption, which changes the conductive properties of the material based on the adsorbed molecule.[1-2]



Dynamics are run for a simulation cell consisting of a periodic zigzag single wall (4,0) CNT surrounded by a monolayer of hydrogen peroxide, with 8 hydrogen peroxides per unit cell of CNT. Simulations are performed on the system under temperatures up to 2000 K, and pressures up to 1000 atmospheres. The system is also examined under time dependent optical excitations, as well as charged states (to simulate exposure to acidic and basic environments). As a result of these reactions, we see formation of epoxide {$C_N + H_2O_2 \rightarrow C_NO + H_2O$}, carbonyl {$C_N + H_2O_2 \rightarrow C_NO + H_2O$}, hydroxyl {$C_N + H_2O_2 \rightarrow C_NOH + OH$}, hydroperoxyl groups {$C_N + 2H_2O_2 \rightarrow C_N{>}OOH + H_2O + OH$}, and CNT hole formation {$C_N + H_2O_2 \rightarrow C_{N-1} + H_2O + CO$}.

These simulations use density functional theory (DFT) with Perdue Burke Ernzerhof (PBE)[3] functional in the Vienna *Ab−initio* Simulation Package (VASP)[4] software. Further work includes in inspection of the conductivity for functionalized carbon nanotubes.

1. Mittal, M.; Kumar, A., Carbon nanotube (CNT) gas sensors for emissions from fossil fuel burning. *Sensors and Actuators B: Chemical* **2014,** *203*, 349-362.
2. Kauffman, D. R.; Star, A., Graphene versus carbon nanotubes for chemical sensor and fuel cell applications. *Analyst* **2010,** *135* (11), 2790-2797.
3. Perdew, J. P.; Burke, K.; Ernzerhof, M., Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996,** *77* (18), 3865-3868.
4. Kresse, G. F., J., 54 (16), 11169-11186. *Physical Review B* **1996,** *54* (169), 11169-11186.