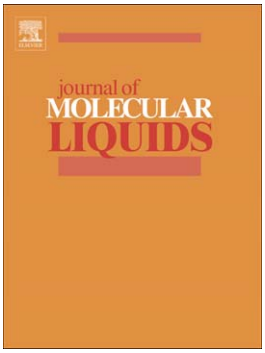

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The effect of solvents on Formaldehyde adsorption performance on pristine and Pd doped on single-walled carbon nanotube using density functional theory

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Abstract

The electronic and structural properties of Pd doped single-walled carbon nanotubes show advantages as new nanocomposies that enable a wide variety of applications as nanosensors, nano storage devices, nanoplatform in biosensors. Our previous research demonstrated that Pd atom loaded onto single-walled carbon nanotubes have been shown that sensitivity of Pd/CNT toward CH_2O in gas phase is twelve times opposed to intrinsic CNT. A detail and widespread study of solvent effects on adsorption of formaldehyde onto pristine single-walled carbon nanotube and Pd loaded on carbon nanotube was performed under density functional theory framework. Based on the results, carbon nanotube showed no obvious sensitivity towards formaldehyde in considered solvents including water, methanol, ethanol, acetone and carbon tetrachloride. Electronic properties of Pd/CNT after CH_2O adsorption were considerably changed. Also, the most and the least adsorption energy were reported in the presence of carbon tetrachloride and methanol from O (O-Pd/CNT) and para (para-Pd/CNT) orientations with -1.174 eV and -0.519 eV adsorption energy respectively. NBO analyses showed in the similar transfers, there was the most strong charge transfer from formaldehyde (O orientation) to Pd/CNT in carbon tetrachloride solution through lone pair of O atom towards lone pair* of Pd site with second-order perturbation energy ($E^{(2)}$) equal 113.345 kJ/mol. These results are representative of strong chemisorption between CH_2O and Pd/CNT in the presence of carbon tetrachloride.