Calculation of the electron affinity properties of the pristine and functionalized adamantane molecules using time-dependent density functional theory (TD-DFT)

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The electron affinity (EA) and electronic structure of the pristine and the functionalized adamantane molecules were determined using the time-dependent density functional theory (TD-DFT) method within local density approximation (LDA). Tertiary hydrogen atoms of the pristine adamantane were replaced with lithium (Li) and sodium (Na) atoms to form the $\text{C}_{10}\text{H}_{16-}\text{NX}_{N}$ structure. We found that the pristine adamantane has a large band gap and show negative electron affinity behavior. In contrast with all functionalized adamantane, it found that Li and Na incorporated in the adamantane structure result their narrower band gap ranging from 0.08 to 1.34 eV. This result suggests the potential applications in optoelectronics in the infrared radiation region which is included the positive electron affinity behavior. The negative electron affinity of the pristine adamantane molecule makes it possible to produce electron emission devices.