عنوان مقاله:
A DFT study of NMR parameters for MgO nanotubes

محل انتشار:
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خلاصه مقاله:
Magnesium oxide nanotubes of finite length are investigated by the Density Functional Theory (DFT) at the B۳LYP/۶-۳۱G (d) level. The (۶, ۰) zigzag and (۴, ۴) armchair of MgO nanotubes were considered and nuclear magnetic resonance properties including isotropic and anisotropic chemical shielding parameters (CSI and CSA) were calculated for ۲۵Mg and ۱۷O atoms of the optimized structures for the first time. The calculated CS parameters indicated that the Mg atoms cause slight changes of electronic environment in the MgONT structures, but the changes for the O atoms are more significant. Results indicated that the zigzag MgONTs could be considered a more reactive .material than the armchair model for interactions with other atoms or molecules

کلمات کلیدی:
Density Functional Theory (DFT), Magnesium Oxide nanotubes, Chemical shielding, Nuclear Magnetic (Resonance(NMR