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Title:	A DFT investigation of the dependence of C13 and F19 CSA parameters on diameter and surface decorated functional groups in F-SWCNTs
Authors:	Kumari, Amrita (/jspui/browse?type=author&value=Kumari%2C+Amrita)
Keywords:	SWCNT Fluorination GIPAW
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Abstract:	The structural characterization of fluorinated zigzag (4,0), (6,0), (8,0) and (10,0) single walled carbon nanotubes (F-SWCNT) has been investigated theoretically using C13 and F19 NMR spectroscopy. The functional groups NHNHCH ₃ , NCH ₂ OH, CH ₂ NHCH ₂ and CH ₂ COOH have been attached covalently in (8,0) F-SWCNT and the corresponding changes in C13 and F19 chemical shift signatures have been examined. The binding energy, charge and bond length variation due to fluorination are reported. A set of isotropic and anisotropic chemical shift variables is deduced from the Gauge Including Projector Augmented Wave (GIPAW) computations of the F19 and C13 nuclei in Pristine and F-SWCNTs. We show that the F19 chemical shift parameters are better structural markers than their C13 counterparts to clearly reveal the nanotube diameter dependency and the type of functional groups which are attached to the fluoronanotubes.
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