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Title:	Guest species trapped inside carbon nanotubes
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Basis sets Density functional External electric fields Guest species
Issue Date:	2009
Publisher:	Elsevier B.V.
Citation:	Chemical Physics Letters, 473 (1-3), pp. 146-150.
Abstract:	Taking the torsional motion of H ₂ O ₂ inside a carbon nanotube as an example, the interaction between the encapsulated guest species and the carbon nanotube has been studied using the density functional theoretical method with the B3LYP functional and the 6-31G ** basis set. Depending upon its orientation inside the nanotube, H ₂ O ₂ binds differently with the nanotube thereby inhibiting the torsional motion in the encapsulated state. The binding of the guest species with the nanotube due to the weak O-H... π interaction is discussed. The polarization of the nanotube because of the guest species suggests that the molecular motion through the nanotube may be influenced by polar solvents and external electric fields.
Description:	Only IISERM authors are available in the record.
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