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**Van der Waal's corrected linear-scaling Density Functional Theory investigation of inner-surface functionalized inorganic nanotubes** JOSHUA ELLIOTT, GILBERTO TEOBALDI, Univ of Liverpool — We report a linear-scaling Density Functional Theory investigation of single-walled open-ended aluminosilicate nanotubes with inner methyl functionalization (AlSiMe NTs). In line with the experimental pore-size distributions,[1] optimization of the AlSiMe NT structure with six different semi-local and non-local van der Waals DFT functionals suggests the presence of a shallow energy-minimum for NTs with 28 to 32 Al-atoms in the NT circumference, resulting in larger diameter than for aluminosilicate (AlSi) NTs. Analysis of the AlSiMe NTs electronic structure reveals the wall-polarization and real-space separation between Valence Band and Conduction Band, characteristic of AlSi NTs.[2] Regardless of the functional, the wall of the AlSiMe NTs are however found to be less polarized than AlSi NTs, with NTs of larger diameter being more polarized. We quantify the effect of the AlSiMe NTs wall-polarization and polarizability on the absolute alignment of the states for adsorbed $H_2O$ molecules inside and outside the tube-cavity. The simulations indicate shifts as large as 2 eV between the $H_2O$-states for molecules adsorbed inside and outside the NT-cavity.

[1] **Phys. Chem. Chem. Phys.**, 13, 744(2011)
[2] **J. Phys. Condens. Mat.**, 21, 195301(2009)

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