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Cation-vacancy and electron-hole relaxation in single-walled aluminosilicate nanotubes: a linear-scaling Density Functional Theory study
EMILIANO POLI, GILBERTO TEOBALDI, Univ of Liverpool — We report a linear-scaling Density Functional Theory (DFT) study of cation-vacancy related defects in single-walled aluminosilicate nanotubes (AlSi NTs), based on the structures derived from solid-state Nuclear Magnetic Resonance.[1] Defect geometry optimization leads to water condensation and modifications to the AlSi NT hydrogen network around the defect sites, leaving no dangling bond. Electronic structure analysis indicates that defect-states are highly localized in real-space and energy, with appearance of shallow and deep occupied defect states above the valence band (VB) edge of the pristine-NT. Electrostatic alignment of the defect states suggests energetically favourable separation of photo-generated electrons and holes on different defects, which may promote defect-centred photochemistry. The peculiar energy alignment of the defect-states is found to be qualitative unaffected by protonation of the defect-sites. These results should be a useful complement to ongoing experimental research in the potential of (alumino)silicate-based nano-porous materials for photocatalysis.[2].

[1]G. Yucelen et al.,**J. Phys. Chem. C.**,116, 17149, 2012
[2]F. Sastre et al.,**J. Am. Chem. Soc.**,133, 17257, 2011

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