Towards Single Strand SnIP

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The diverse structure of SnIP[1] on the nanoscale, ranging from strong covalent bonding to weak van der Waals interactions, and the large anisotropy offers a substantial potential for applications in energy conversion and solar fuel production. However, a suitable way to separate the pairwise occurring strands into particles smaller than five to ten shells of hexagonally stacked, right (p) and left (m) handed double helices is still lacking. Thinking about a bottom-up approach, one can imagine using single walled carbon nanotubes (SWCNTs) as a suitable matrix to grow separated SnIP helices, which might even be influenced by the chirality of the SWCNTs. First three different nanotubes were chosen by diameter, length of 1D unit cell and the electronic properties. Optimizations were performed with the Crystal17 program package on the GGA – level with the PBE functional and the Grimme D3 correction.

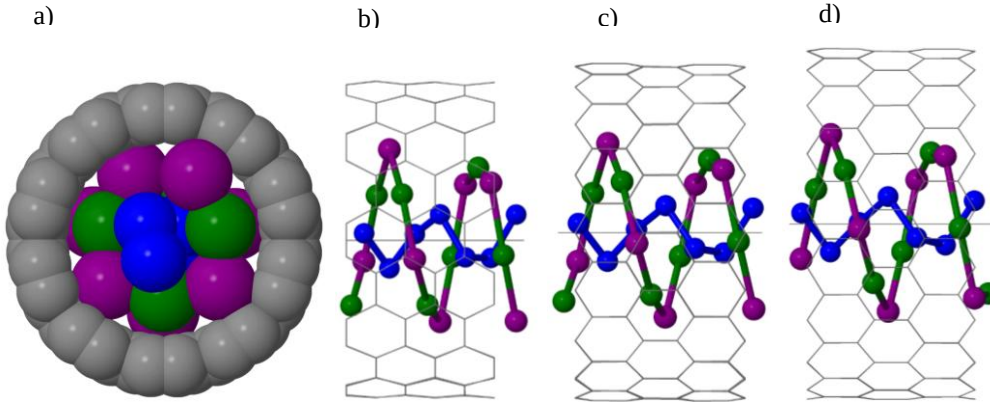

Figure 1: Optimized structures of a) SnIP in SWCNT (10,10) drawn in space filling mode along the *a* axis; b) SnIP in a SWCNT (10,10) with diameter dT = 13.7 Å and view onto axis *a*; SnIP in SWCNT (18,0) with dT = 14.2 Å and view onto axis *a*; d) SnIP in SWCNT (19,0) with dT = 15.1 Å and view onto axis *a*.

In Figure 1a) and 1b) SnIP can be seen in the metallic SWCNT (10,10), where the space filling view shows the interaction between SWCNT and SnIP happens mainly between iodine and carbon atoms. The calculations show weak but definitely relevant interactions in these hybrid structures of SnIP. The semimetallic SWCNT (18,0) (Figure 1c) and the semiconducting SWCNT (19,0) (Figure 1d) is shown. Electronic structures are predominantly determined by the chosen SWCNTs, which are much more rigid than SnIP.

1. Baumgartner, M.; Weihrich, R.; Nilges, T., *Chemistry – A European Journal* **2017**, *23* (26), 6452-6457.