Crystallography and Functional Evolution of Atomically Thin Confined Nanowires

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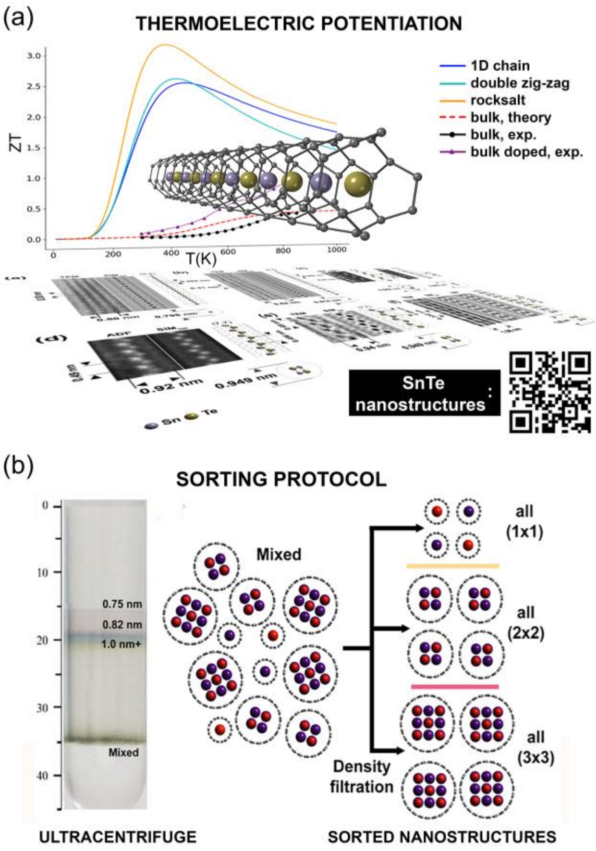

Fig. 1 (a) *Effect of Nanostructuring SnTe on the Seebeck Coefficient (ZT) vs. the bulk phase. Plot is ZT vs. T(K) Insets include 1D SnTe inside a (6,6) SWCNT and (bottom) the observed nanostructures included in the plot [3].* ***(b)*** *Nanostructuring creates differences in both density and electronic structure which means that thin films can be created by 'sorting' mixed samples in which only one structure type exists in a fraction. The ZT of a single nanostructure can then be tested in isolation (cf. panel* ***(a)****).*

Encapsulated nanowires can be as small as a single atom in width and are the smallest one-dimensional materials. Their simplicity and robustness makes them ideal platforms for the study of fundamental properties of matter, such as phase transformations and the energetics of confined crystal structure formation. Carbon nanotubes are the ideal encapsulation template, and enable the observation of crystalline/non-crystalline transitions and molecular ordering either into chains or discrete species. These materials have tested, and continue to test, the state of the art in atomic-resolution electron microscopy and their associated spectroscopies. The extremely small size also lends these materials to *ab initio* (or *a posteriori*) theoretical investigations whereby their stability, electronic properties and properties can all be studied. This work is leading to ground-breaking and transformative new studies of the exotic physics of atomically-thin 1D wires, including the physical realisation of the Peierls distortion, novel phonon optics and, most recently, the spectacular modification of thermal properties [1-3, Fig. 1(a)]. A further recent innovation is the observation and study of confined phase transformations at the smallest volume scale ever attempted, an essential precursor to the determination of the smallest scale that we can write information by the technique of PC-RAM [4-5].

Forming nanowires on such small physical scales presents unique and benchmarking challenges for high performance electron microscopy and spectroscopy as these must perform at or close to the level of single atom sensitivity. The student will contribute to an EPSRC-funded experimental project on the synthesis and characterisation of Atomically Regulated Nanowires by state-of-the-art electron microscopy and other characterisation methodologies, including Raman and ultrafast terahertz spectroscopies. A major goal will be to determine the unique physical properties of atomically-thin nanowires in several respects that are quantitative: (i) in terms of their 3D crystallography; (ii) in terms of their local electronic environment (i.e. *vis-a-vis* bonding and atomic potentials); (iii) in terms of their emergent macroscopic electronics, conductivity and optoelectronic properties. The student will also interact with Project Partners in Oxford (ePSIC at the Diamond Light Source), Southampton, Warsaw, Vienna, Pau and Beijing, with the opportunity to travel to some of these Partners. Interested applicants should contact j.sloan@warwick.ac.uk (Tel. 02476 523392) or j.lloyd-hughes@warwick.ac.uk.

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