Abstract Submitted
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The II-VI nanostructure zoo PHILIP LINDAN[1], School of Physical Sciences, University of Kent, SAMANTHA LISTER, School of Physical Sciences, University of Kent — We present predictions of a completely new family of nanotubes, related nanostructures and fullerene-like cages formed from the II-VI semiconductor mercury telluride. Our predictions are supported by first-principles calculations on the structures. The structures are remarkable in several ways: They are all more stable than the planar form of HgTe from which they are formed; they are radically altered from the tetrahedral bulk forms, and a strong interaction with the electronic structure results in a semimetal-semiconductor transformation; and for the larger armchair tubes isomerisation leads to striking structures formed from heavy modification of the tube, accompanied by large changes in the bandgap. For the nanotubes two simple rules for preferred coordination of Hg and the Hg-Te-Hg bond angles explain the structural stability of the nanotubes, and the formation of their exotic isomers. The cage structures are based upon the Archimedean and Platonic solids, where key requirements in terms of numbers of vertices, number of triangular faces and their connectivity determine the viable subset of structures.

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