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Nanostructured topological state in bismuth nanotube arrays: Inverting parity symmetry of molecular orbitals[1] KYUNG-HWAN JIN, Department of Materials Science and Engineering, University of Utah, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, FENG LIU, Department of Materials Science and Engineering, University of Utah — The topological order of a solid material is linked to its band topology of Bloch states, hence a topological material is referred to a crystalline material with long-range translational order. Consequently, so far there are only very few studies of topological phases in nanostructured materials. We demonstrate a new class of nanostructured topological materials that exhibit topological quantum phase arising from nanoscale structural motifs. Based on first-principles calculations, we show that an array of bismuth nanotubes (BiNTs), a superlattice of BiNTs with a periodicity in the order of tube diameter, behaves as a nanostructured two-dimensional (2D) quantum spin Hall (QSH) insulator, as confirmed from the calculated band topology and 1D helical edge states. The underpinning mechanism of QSH phase in the BiNT array is revealed to be inversion of parity symmetry of molecular orbitals of constituent nanostructural elements in place of atomic-orbital band inversion. The quantized edge conductance of QSH phase in BiNT array can be more easily isolated from bulk contributions and their properties can be highly tuned by tube size and chirality, representing distinctive advantages of nanostructured topological phases.

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