Abstract Submitted
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The electronic and structural properties of SnO_2 nanoparticles doped with antimony and fluorine[1] MINJUNG KIM, University of Texas at Austin, NOA MAROM, Tulane University, SCOTTY BOBBITT, JAMES R. CHELIKOWSKY, University of Texas at Austin — Transparent conducting oxide (TCO) materials are important owing to their broad industrial applications such as optoelectronic devices and photovoltaics. The most widely used TCO material is In-doped tin oxide (ITO), but In is not abundant in nature. Sb- and F-doped tin oxide nanoparticles are considered as a good candidate of ITO as they have been successfully synthesized. The electronic properties of these nanoparticles depend on the impurity species, the nanoparticle size and shape. We present electronic structure calculations on Sb- and F-doped tin oxide nanoparticles by employing real-space pseudopotential calculations based on density functional theory. We examine the impurity formation energies and electron binding energies with respect to the size of the nanoparticle and the location of the impurity site.

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James Chelikowsky
University of Texas at Austin

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