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A novel nanometric cubic phase in monochalcogenide semiconductors – theory and experiment

A new nanometric cubic binary phase has been synthesized in the tin monoselenide and monosulfide systems, π-SnSe, π-SnS, as cube shaped nanoparticles. This new phase has unusual structural properties reflected in a large, 64-atom unit cell and promising optical properties due to the larger band gap and non-centrosymmetric structure of the crystal. It is also environmentally advantageous. This exciting discovery has already led to the publication of over 25 studies in less than 2 years. However, interpretation of the structure, bonding, stability and electronic properties has proven challenging. By introducing by ab-initio density functional calculations the structure, atomic positions and band gaps of these phases were determined and found to be in very good agreement with experimental measurements. Advanced theoretical studies including density functional calculations of the phonon spectrum that determined these phases to be mechanically stable and energetically close to competing structures such as rock salt and orthorhombic. Furthermore theory predicts that the monochalcogenides will exhibit other, as yet experimentally undiscovered, novel phases with promising properties. This study overview the latest results of our calculations and experimental studies.

Biography

Guy Makov is an Associate Professor of Materials Engineering at Ben-Gurion University of the Negev and his research interests is in Materials Physics. He has completed his BSc in Chemistry; PhD in Chemical Physics at Tel Aviv University and Post-doctorate in Computational Materials Physics at Cambridge University and FZ Julich. His research aims to understand materials behavior under extreme conditions of size, temperature and pressure from a physical viewpoint, in particular electronic structure, equilibrium properties and response to mechanical deformations or irradiation. His areas of specific interest include semiconductor nanoparticles and the liquid state, phase diagrams, dislocations, defects and microstructure in metals.

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