Researchers make theoretical prediction of 2-D semiconductor tin dioxide

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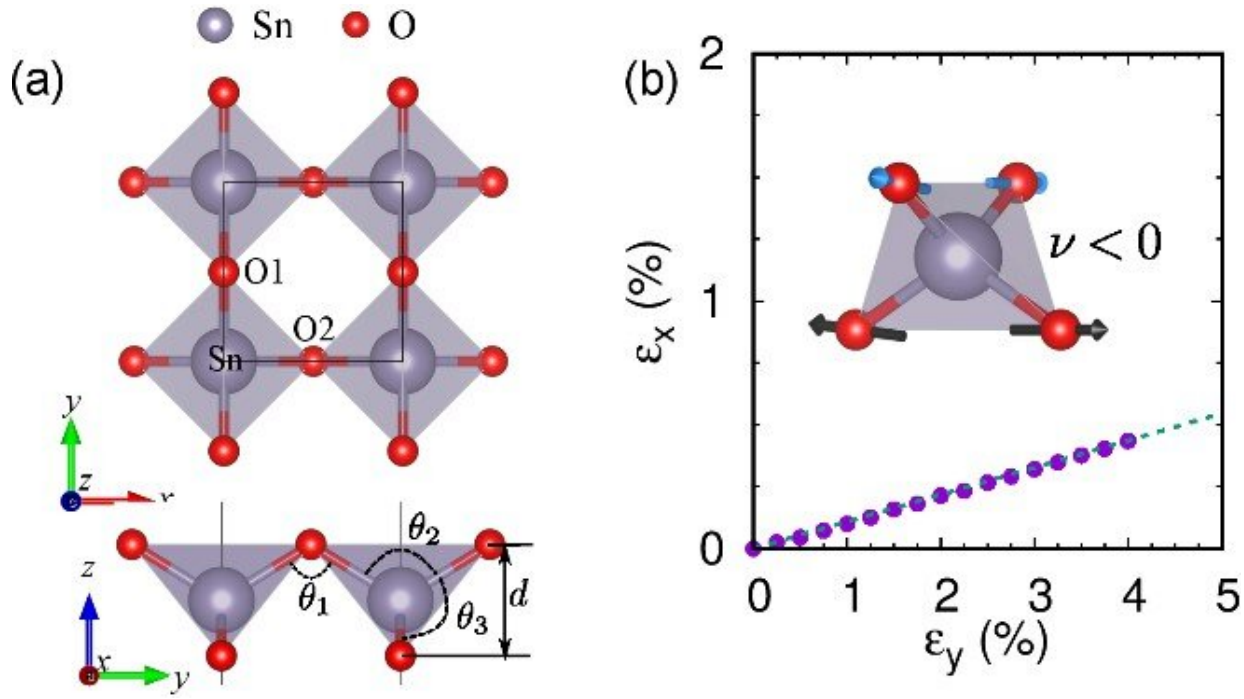

Fig. 1. (a) The atomic structure of a 2D δ-SnO2 monolayer. (b) The strain in the x direction resulting from an applied tensile strain in the y direction. Credit: JIANG Peng

Recently, Prof. Zheng Xiaohong's research group from the Institute of Solid State Physics (ISSP) of the Hefei Institute of Physical Science (HFIPS) predicted a new two-dimensional (2-D) tin dioxide (SnO_2) monolayer phase (P-4 m^2) via first-principles calculations.

Bulk SnO_2 is an important n-type wide-bandgap (~3.6 eV) semiconductor and is widely used as electrode materials, chemical sensor components, etc. but systematic study of possible tin oxide phases in 2-D is still missing. In particular, given the claims of magnetism in SnO_2 thin films, it is worth investigating whether a stable SnO_2 2-D phase can be synthesized or magnetism can be induced.

In this research, the researchers provided direct evidence of a stable and new 2-D phase of SnO_2 (δ- SnO_2) with auxetic properties based on density functional theory method, which was impressive for its negative in-plane Poisson's ratio and high electron mobility.

In addition, they found double Mexican-hat-like band edges near the Fermi level presented by the valence band structure of SnO_2 and therefore a ferromagnetic phase transition and half-metallic ground state could be induced by hole doping within a very wide concentration range.

They also proved that SnO_2 monolayer could be tuned to be either an XY magnet or an Ising one, with a magnetic critical temperature above room temperature at proper hole concentrations.

All the above findings indicated that the predicted 2-D phase of SnO_2 provided a new example of rare p-type magnetism and a potential candidate material for spintronic applications.

More information: Peng Jiang et al. Computational prediction of a two-dimensional semiconductor SnO_2 with negative Poisson's ratio and tunable magnetism by doping, *Physical Review B* (2020). DOI: 10.1103/PhysRevB.102.195408

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