Researchers make theoretical prediction of 2-D semiconductor tin dioxide

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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 ($\sim$3.6 eV) semiconductor and is widely used as electrode materials, chemical sensor components, etc. but systematic study of possible tin oxide phases in 2-D is still missing. In particular, given the claims of magnetism in SnO$_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$_2$ (?-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.


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