Scientists unravel new insights into promising semiconductor material

September 8 2017

Researchers from the National University of Singapore (NUS) have established new findings on the properties of two-dimensional molybdenum disulfide (MoS_2), a widely studied semiconductor of the future.

In two separate studies led by Professor Andrew Wee and Assistant Professor Andrivo Rusydi from the Department of Physics at the NUS Faculty of Science, the researchers uncovered the role of oxygen in MoS_2, and a novel technique to create multiple tunable, inverted optical band gaps in the material. These novel insights deepen the understanding of the intrinsic properties of MoS_2 which could potentially transform its applications in the semiconductor industry.

Researchers from the National University of Singapore have established new findings on the properties of two-dimensional molybdenum disulfide (MoS^2), a widely studied semiconductor of the future.

The studies were published in prestigious scientific journals *Physical Review Letters* and *Nature Communications* respectively.

MoS_2—an alternative to graphene

MoS_2 is a semiconductor-like material that exhibits desirable electronic and optical properties for the development and enhancement of transistors, photodetectors and solar cells.

Prof Wee explained, "MoS_2 holds great industrial importance. With an atomically thin two-dimensional structure and the presence of a 1.8eV energy band gap, MoS_2 is a semiconductor that can offer broader applications than graphene which lacks a band gap."

Presence of oxygen alters the electronic and optical properties of MoS2

In the first study published in *Physical Review Letters* on 16 August 2017, NUS researchers conducted an in-depth analysis which revealed that the energy storage capacity or dielectric function of MoS_2 can be altered using oxygen.

The team observed that MoS2 displayed a higher dielectric function when exposed to oxygen. This new knowledge shed light on how adsorption and desorption of oxygen by MoS2 can be employed to modify its electronic and optical properties to suit different applications. The study also highlights the need for adequate consideration of extrinsic factors that may affect the properties of the material in future research.

The first author of this paper is Dr Pranjal Kumar Gogoi from the Department of Physics at NUS Faculty of Science.

MoS2 can possess two tunable optical band gaps

In the second study published in *Nature Communications* on 7 September 2017, the team of NUS researchers discovered that as opposed to conventional semiconductors which typically have only one optical band gap, electron doping of MoS2 on gold can create two unusual optical band gaps in the material. In addition, the two optical bandgaps in MoS2 are tunable via a simple, straight forward annealing process.

The research team also identified that the tunable optical band gaps are induced by strong-charge lattice coupling as a result of the electron doping.

The first author of this second paper is Dr Xinmao Yin from the Department of Physics at NUS Faculty of Science.

The research findings from the two studies lend insights to other materials that possess similar structure with MoS_2.

"MoS2 falls under a group of material known as the two-dimensional transitional metal dihalcogenides (2-D-TMDs) which are of great research interest because of their potential industrial applications. The new knowledge from our studies will assist us in unlocking the possibilities of 2-D-TMD-based applications such as the fabrication of 2-D-TMD-based field effect transistors," said Asst Prof Rusydi.

Leveraging the findings of these studies, the researchers will apply similar studies to other 2-D-TMDs and to explore different possibilities of generating new, valuable properties in 2-D-TMDs that do not exist in nature.

More information: Pranjal Kumar Gogoi et al. Oxygen Passivation Mediated Tunability of Trion and Excitons in MoS2, *Physical Review Letters* (2017). DOI: 10.1103/PhysRevLett.119.077402

Xinmao Yin et al. Tunable inverted gap in monolayer quasi-metallic MoS2 induced by strong charge-lattice coupling, *Nature Communications* (2017). DOI: 10.1038/s41467-017-00640-2

Provided by National University of Singapore