Contribution ID: **218** Contribution code: **S06-CMPSP-219** Type: **Poster presentation**

Midgap state in silicon carbide monolayer induced by atom adsorption

Tuesday 30 August 2022 18:00 (1h 30m)

The recent synthesis of two-dimensional (2D) silicon carbide (SiC) [1] experimentally proved the existence of 2D carbides, a new class of semiconducting materials with the honeycomb structure. Considering the point defects, one of the simplest structural deformations in 2D materials, we examined the prospect of employing them for the band-gap engineering of a SiC monolayer. Applying density functional theory, we found that in a free-standing SiC layer, out of the plane deformation of a single silicon atom creates a new midgap state otherwise not present in a perfectly flat sheet [2]. Additionally, upon a continuous displacement of the Si atom in the direction perpendicular to the layer, the midgap state shifts from the top of conduction to the bottom of the valence band. A tight-binding model reproduces a qualitative understanding of midgap state energy shift. The inspected deformations can be realized by the adsorption of suitable metal atoms. We chose lithium (Li) [3] and calcium (Ca) atoms since they strongly bind to the SiC and donate one and two electrons, respectively. Furthermore, we found that the midgap state induced by atoms in SiC is filled by one electron in the case of Li and two electrons with opposite spin in the case of Ca adatoms. We demonstrated that the electronic charge transfer from the adsorbate to the SiC alters both its structural and electronic properties to a much greater extent than in other known 2D honeycomb crystals.

References

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Session Classification: Poster session

Track Classification: Scientific Sections: S06 Condensed Matter Physics and Statistical Physics