



Contribution ID: 38

Type: Invited Oral

Defects physics in emergent 2D material SnSe with binary black phosphorus lattice

Wednesday, 15 August 2018 16:30 (30 minutes)

In this talk, we will show the pronounced effects of various defects in determining the physical properties of the emergent 2D material SnSe with binary black phosphorus lattice. SnSe has been reported with record-breaking thermoelectric conversion efficiency very recently. However, to date a comprehensive understanding of the electronic structure and most critically, the self hole-doping mechanism in SnSe is still absent. We for the first time fully unfold the highly anisotropic electronic structure of SnSe by angle-resolved photoemission spectroscopy, which reveals a unique pudding-mould-shaped valence band with quasi-linear energy dispersion. We prove that p-type doping in SnSe is extrinsically controlled by local phase segregation of SnSe₂ microdomains via interfacial charge transferring. The multivalley nature of the pudding-mould band is manifested in quantum transport by crystallographic axis-dependent weak localisation and exotic non-saturating negative magnetoresistance. Strikingly, quantum oscillations also reveal 3D Fermi surface with unusual inter-layer coupling strength in p-SnSe, in which individual monolayers are interwoven by peculiar point dislocation defects. The fingerprinting pudding-mould multivalley band structure is well reserved in bismuth-doped n-type SnSe, which suggest the feasibility of an all-SnSe functioning device.

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Session Classification: Speaker Sessions and Seminars

Track Classification: Electronic Materials and Processing