

Poster-2-31

An Ab Initio Study of Superconductivity in Mono- and bilayer Molybdenum disulfideWouter Bos*MSc student*

The two-dimensional electron doped form of molybdenumdisulfide (MoS₂) exhibits superconducting properties around liquid-helium temperatures. Ion-liquid gating experiments have shown a layer dependent increase in critical temperature from 1-2 Kelvin (K) to around 7 K in the transition from monolayer to bilayer MoS₂ converging to 10 K in bulk MoS₂ [1, 2, 3]. In this thesis an attempt has been made to increase the understanding of conventional superconductivity in doped monolayer and bilayer MoS₂ by using state of the art ab initio techniques such as, DFT, DFPT, Wannier interpolation and Eliashberg theory. These techniques were ultimately used to predict trends in critical temperatures differentiating by layer thickness, spin polarization and charge distribution. The valley and band resolved electron-phonon coupling strengths were calculated using a self-written Python script, which showed electron occupation of the Q-region to be crucial to superconductivity in bilayer MoS₂.

[1] Yajun Fu et al. "Gated tuned superconductivity and phonon softening in monolayer and bilayer MoS₂". In: npj Quantum Materials 2 (1 Dec. 2017). ISSN: 23974648. DOI: 10.1038/s41535-017-0056-1.

[2] Davide Costanzo et al. "Gate-induced superconductivity in atomically thin MoS₂ crystals". In: Nature Nanotechnology 11 (4 Apr. 2016), pp. 339-344. ISSN: 17483395. DOI: 10.1038/nnano.2015.314.

[3] Davide Costanzo et al. "Tunnelling spectroscopy of gate-induced superconductivity in MoS₂". In: Nature Nanotechnology 13 (6 June 2018), pp. 483-488. ISSN: 17483395. DOI: 10.1038/s41565-018-0122-2.