Electronic Structure of Misfit Layered Compound $(LaSe)_{1.14}(NbSe_2)_2$ from First-Principles

Jozef Haniš and Martin Gmitra

Institute of Physics, Pavol Jozef Šafárik University in Košice, Park Angelinum 9, 04001 Košice, Slovak Republic

Corresponding author: jozef.hanis@student.upjs.sk

Abstract. Transition metal dichalcogenides (TMDs) reveal possess several interesting physical properties including superconductivity with in-plane upper critical magnetic fields much higher than the Pauli limit explained be means of unconventional Ising pairing mechanisms [1]. Misfit layered $(LaSe)_{1.14}(NbSe_2)_2$ is a stack of TMDC layers intercalated by the LaSe layers. Those systems are superconductors even they are arranged in different vertical stackings [2,3]. We discuss electronic structure from density functional theory calculations for misfit layered $(LaSe)_{1.14}(NbSe_2)_2$ compound for different bulk stacking and slab configurations, calculate quasiparticle interference in normal state using T-matrix approach [4] by means of tight-binding model [5] fitted to the first-principles calculations relevant for Fourier-transform scanning tunneling spectroscopy.

This work was supported by the project CEDAMNF, reg. no. CZ.02.1.01/0.0/0.0/15_003/ and VEGA Grant No. 1/0105/20.

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