Contribution ID: **241** Type: **Oral**

Computational Simulations Applied to Kagome GdV6Sn6

In this talk, I will present a recent computational study applied to Kagome GdV6Sn6 nanomaterials. We compared results about the Fermi surface and the Haas van Alphen quantum oscillations with experimental data. The spin-orbit effect and high electron correlation due to f-orbitals are mandatory to reach a good agreement with the experiment. The angle-dependent dHvA oscillation frequencies indicate that the smaller pockets of the Fermi surface have almost 3D character, whereas the bigger pockets are mostly two-dimensional. The comparison of the observed frequencies with the electronic structure calculations indicates that the heavier masses correspond to saddle point-like features of electronic structure at M point contributed by and bands. Our work reveals the features of the Fermi surface containing heavier fermions originating from saddle points in the electronic structure at the M point inherent to the Kagome lattice.

Keywords

Kagome, Flat bands, Spin-orbit coupling

Reference

C. Dhital, et al., Accepted for publication in Physical Review B, 2024.

This work was supported by

J.G.S acknowledges DGAPA-UNAM project IG101124. Calculations were performed in the DGCTIC-UNAM Supercomputing Center project LANCADUNAM-DGTIC-368, LNS-BUAP project 202201042N, and THUBAT KAAL IPICYT supercomputing center project TKII-JGSA001. J.G.S. also acknowledges A. Rodriguez-Guerrero and E. Murillo for useful discussions and technical assistance.

Author approval

I confirm

Author will attend

I confirm

Author: Dr GUERRERO SANCHEZ, Jonathan (Centro de Nanociencias y Nanotecnología, UNAM)

Presenter: Dr GUERRERO SANCHEZ, Jonathan (Centro de Nanociencias y Nanotecnología, UNAM)

Session Classification: NANOSTRUCTURES

Track Classification: Nanostructures