XXIII Simposio Chileno de Física
Chile, 22-24 noviembre 2022 Física de la Materia Condensada

High-temperature phonon-mediated superconductivity in monolayer $Mg_2B_4C_2$

S Singh[1*], AH Romero [2], JD Mella[3], V. Eremeev[4], E. Munoz[5], AN Alexandrova[6], KM Rabe[7], D Vandervilt[8], F. Munoz[3,4*]

[1] University of Rochester, New York, USA.
[2] West Virginia University, Morgantown, West Virginia, USA
[3] Universidad de Chile, Santiago, Chile
[4] Universidad Diego Portales, Santiago Chile
[5] Pontificia Universidad Católica de Chile, Santiago, Chile
[6] University of California, Los Angeles, USA
[7] Rutgers University, New Jersey, USA
[8] Center for the Development of Nanoscience and Nanotechnology, CEDENNA, Santiago, Chile

*fvmunoz@gmail.com

Resumen

A two-dimensional material – $Mg_2B_4C_2$, belonging to the family of the conventional superconductor MgB_2, is theoretically predicted to exhibit superconductivity with critical temperature Tc estimated in the 47–48 K range without any tuning of external parameters such as doping, strain, or substrate-induced effects. The origin of such a high intrinsic Tc is ascribed to the presence of strong electron-phonon coupling and large density of states at the Fermi level. Our calculations confirm the stability of 2D $Mg_2B_4C_2$[1]

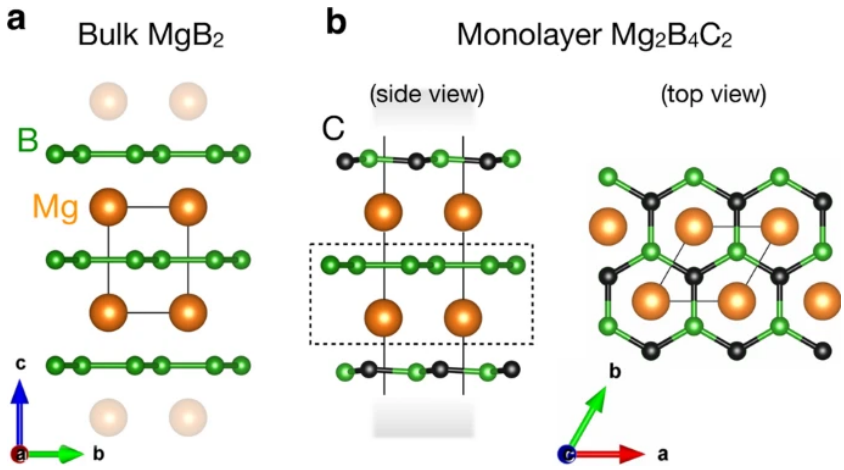

Figura 1: (a) Bulk MgB_2, and (b) side and top views of monolayer $Mg_2B_4C_2$ (Mg: orange, B: green, C: black). Solid black lines mark the unit cell boundaries, and shaded gray areas represent vacuum in the left panel of (b). The region marked by dashed black lines in (b) can be arbitrarily repeated.

Agradecimientos: Fondecyt Grant No. 1191353, Center for the Development of Nanoscience and Nanotechnology CEDENNA AFB180001, and Conicyt PIA/Anillo ACT192023This research was partially supported by the supercomputing infrastructure of the NLHPC (ECM-02)

Referencias

[1] Singh, S., Romero, A.H., Mella, J.D. et al. High-temperature phonon-mediated superconductivity in monolayer Mg2B4C2. npj Quantum Mater. 7, 37 (2022).