Lifshitz transition in cI16 Li at high pressures: Unfolding first-principles Fermi surfaces

CHIA-HUI LIN, TOM BERLIJN, WEI KU, Brookhaven National Laboratory/ Stony Brook University — The Fermi surface topology of cI16 Li is investigated using the recently developed first-principles band structure unfolding method [1]. The resulting unfolded Fermi surfaces display a clear Lifshitz transition at 47 GPa, explaining the anomalous change of superconducting transition temperature [2]. The unfolded Fermi surfaces also reveal a more complete picture of the driving force of the cI16 phase starting at 39 GPa [3]. In addition to the previously proposed “nesting” effect [3] along [1\frac{1}{2}1], both [100] and [\frac{1}{2}\frac{1}{2}0] wavevectors are found to contribute significantly to the structural instability as well, due to their large phase space, a more effective effect in 3D. We expect a wide range of applications of this Fermi surface unfolding method to the study of high pressure electronic structure.