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Lifshitz transition in *cI*16 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 reveals 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 $[1\frac{1}{2}\frac{1}{2}]$, 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.

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[2] S. Deemyad and J. S. Schilling, Phys. Rev. Lett. **91**, 167001 (2003)
[3] M. Hanfland et al, Nature **408**, 174 (1998)

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