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Complexity and Pressure Induced Fermi Surface Deformation in Lithium AITOR BERGARA, ALVARO RODRIGUEZ-PRIETO, University of the Basque Country (UPV/EHU) and Donostia International Physics Center (DIPC), V.M. SILKIN, Donostia International Physics Center (DIPC), UPV/EHU AND DIPC TEAM — Recently reported structural complexity and high temperature superconducting transition in lithium under pressure has increased the interest in light alkalis, otherwise considered as simple and well known systems under normal conditions. In this work we present an analysis of the pressure induced Fermi surface deformation in lithium and its relation to the observed complexity. According to our calculations, the Fermi surface becomes increasingly anisotropic with pressure and at around 8 GPa it contacts the Brillouin zone boundary, which preludes the bcc to fcc phase transition. Furthermore, at around 30 GPa, besides the increasing necks in the Fermi surface along the fcc ΓL direction, it develops an extended and well defined nesting in the ΓW direction, which enhances the electronic response for the nesting momentum and induces an strong phonon softening along the ΓK. The increasing electron-phonon coupling associated to this softening, besides preluding the transition to complex structures, also provides a better understanding of the observed superconducting transition in lithium at around the same pressure range.

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