Pressure Induced Complexity in Light Alkalies

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Recently reported correlated structural complexity[1] and enhanced temperature superconducting transition[2] in lithium under pressure have increased the interest in light alkalies, otherwise considered as simple and well known systems under normal conditions. Strong modification of bonding and electronic properties in lithium under pressure[3] becomes the origin of its strong departure from the classical nearly free electron like model. In this talk 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 8 GPa contacts the Brillouin zone boundary inducing a Hume-Rothery mechanism explaining the *bcc-fcc* transition. Around 30 GPa increasing cooper-like necks and an extended nesting are observed in the Fermi surface in the *fcc* phase, enhancing the electronic susceptibility response function and inducing a strong phonon softening[4]. This softening, besides preluding the transition to complex structures and providing a better understanding of the observed superconductivity[5], is expected to induce other yet unexplored anomalies in compressed lithium. Additionally, we will propose the existence of a new low energy undamped interband collective mode[6] arising with the *bcc-fcc* structural transition in lithium under pressure, which is expected to induce an abrupt plasma edge in the experimentally observable reflectivity and also affect electronic correlations at low energies.

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