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Strong Electron-Phonon Coupling in Elemental Metals Under Pressure ZHIPING YIN, WARREN PICKETT, Physics Department, UC Davis — The superconductivity of yttrium with T_c=20K at 115 GPa has been confirmed by strong electron-phonon coupling obtained using linear response methods. The increase of T_c under pressure mainly comes from the increasingly strong coupling to the transverse modes at all high-symmetry zone boundary points X, K, and L. Evaluation of the electron-phonon spectral function shows a very strong increase with pressure of coupling strength in the 2-8 meV range, but with an accompanying steady increase in the 8-20 meV range.The superconductivity of Ca under pressure, however, is a challenge. While other elemental superconductors are usually close-packed, Ca is simple cubic (SC) at pressure between 30 GPa and 109 GPa, and its T_c increases significantly in this pressure range, and goes to 23 K at 109 GPa (25 K at 161 GPa), making Ca the highest T_c superconductor among elements. From linear response calculations we find the harmonic frequencies are unstable over a large portion of the zone for a wide range of pressure in the SC phase. We present calculational results and discuss possibilities, which include the likely stabilization of the SC structure by large anharmonic contributions to the lattice dynamics.

Zhiping Yin
Physics Department, UC Davis

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