Calculation of electron-phonon coupling in Arsenic under pressure[1] KEVIN T. CHAN, MARVIN L. COHEN, Dept. of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Elemental As undergoes a structural transformation from a rhombohedral A7 phase to a simple cubic (sc) phase at around 25 GPa as pressure is increased. At pressures near this phase transformation, As is superconducting, with a maximum superconducting transition temperature T_c of about 2.5 K. Experiments indicate that this maximum T_c occurs at the transition pressure for structural transformation, and the increase in T_c as the transition pressure is approached has been attributed to phonon softening. In this work, we calculate from first principles the electronic structure, phonon dispersions, and electron-phonon coupling constant λ for As in the A7 and sc phases at various pressures near the A7 to sc transition. Using these detailed quantitative calculations, we explain the trends in T_c as function of pressure in terms of phonon softening, electronic density of states, and electron-phonon matrix elements. We discuss the implications of these results for finding new superconducting materials.

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