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DFT Calculations for the Uranium EOS CARL GREEFF, SCOTT CROCKETT, SVEN RUDIN, JOHN WILLS, Los Alamos National Laboratory —
We present results of density functional theory calculations on the Uranium equation of state. We examine the influence of approximations for the exchange-correlation functional and spin-orbit interaction, as well as numerical methods such as pseudopotentials. We compare calculated properties, such as static lattice energies and electronic specific heats, to their empirically derived counterparts.

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