

Abstract Submitted
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Correlation induced phase transition in fcc Pu SHAO-PING CHEN,
Los Alamos National Laboratory — The density functional theory calculations (GGA+U) of fcc Pu indicate that as the Hubbard on-site Coulomb repulsion U increases the fcc Pu system goes through a sharp phase transition. Accompanying this transition are sharp drops of the bulk moduli, and large values and even negative values of pressure derivatives of the bulk moduli. Some evidence of these effects were consistent with current experimental observations.

Shao-Ping Chen
Los Alamos National Laboratory

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