

Abstract Submitted
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Electronic structure and superconductivity in rare and not so rare monatomic materials LANE NIXON, DIMITRIS PAPACONSTANTOPOULOS, George Mason University — We have calculated the electronic structure of Eu and P for different crystal structures and volumes using the augmented-plane wave method with both the local-density and generalized-gradient approximations. Europium calculations used a frozen-core approximation with a semi-empirical shift of the logarithmic derivatives which moves the 5f states below the valence bands. This shift of the localized f-states yields the correct europium phase ordering with lattice parameters and bulk moduli in good agreement with experimental data. The calculated superconductivity properties under pressure for the bcc and hcp structures are also found to agree with and follow a T_c trend similar to recent measurement by Debessai et al.¹ The phosphorus phase ordering has been found for high-symmetry allotropes, with lattice parameters and bulk moduli in good agreement with experimental data. The calculated superconductivity properties under pressure for the simple cubic structure is found to agree with measurements and we predict the bcc phase as a high pressure superconductor.

¹M. Debessai, T. Matsuoka, J. J. Hamlin, J. S. Schilling, and K. Smimizu, Phys. Rev. Lett. 102, 197002 (2009).

Lane Nixon
George Mason University

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