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Electronic structure and properties of lanthanum LANE NIXON, DIMITRIOS PAPACONSTANTOPOULOS, George Mason University — The total energy and electronic structure of lanthanum have been calculated in the *bcc*, *fcc*, *hcp* and *dhcp* structures for pressures up to 50 GPa. The full potential linearized-augmented-planewave method was used with both the local-density and general-gradient approximations. The correct phase ordering has been found, with lattice parameters and bulk moduli in good agreement with experimental data. The GGA method shows excellent agreement overall while the LDA results show larger discrepancies. The calculated strain energies for the *fcc* and *bcc* structures demonstrate the respective stable and unstable configurations at ambient conditions. The calculated superconductivity properties under pressure for the *fcc* structure are also found to agree well with measurements. Both LDA and GGA, with minor differences, reproduce well the experimental results for T_c.

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