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Osmium under high pressure: a fully relativistic first-principles study of the structural and electronic properties. ALBERTO RUBIO-PONCE, Departamento de Ciencias Basicas, UAM-Azacapatzalco, Mexico., ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — Recently, there has been much interest in the high-pressure properties of Os after that the first bulk modulus measurement was made only four years ago. It is important to mention that to date, the phase diagram of Os is unknown. In the present work, we have studied the structural and electronic properties of Os using the full-potential LAPW method and the GGA for the exchange-correlation functional. The calculations were performed including the spin-orbit coupling which is important for heavy metals like Os. The total-energy as a function of the cell volume was computed assuming the hcp, fcc, and ω structures, for compressions up to 65% of the equilibrium volume. In contradiction with the previous non-relativistic LDA-calculation, we find that Os in the hcp phase have lower energy than the fcc and ω structures. The hcp structure remains stable for pressures up to 400 GPa and not structural transition to the fcc or ω phase was found. Nevertheless, from the analysis of the band structure, we find an electronic topological transition induced by pressure at the high-symmetry point L, where three bands cross the Fermi level upon compression.

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