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Wannier-Like Functions of Cesium Under High Pressure EVA ZUREK, Max Planck Institute for Solid State Research, OLE KROGH ANDERSEN, Max Planck Institute for Solid State Research — At ambient pressures cesium metal is found in the body centered cubic structure. At higher pressures, it undergoes a series of phase transitions which are accompanied by an electronic transition of the valence s electron to d-like states. We first of all propose a procedure which may be used to obtain Wannier-like functions for metallic systems using the newly developed NMTO (Muffin Tin Orbitals of order N) method. Wannier-like orbitals for a subset of the experimentally determined crystal structures of cesium are calculated. The electron density obtained from these orbitals is compared with that obtained from standard LMTO calculations. These orbitals give clear evidence of the electronic transition: they are primarily s-like at ambient volumes and display an increasing amount of d-character for structures found at higher pressures.

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