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Three Aspects of the Computation of Electronic Structures of Metals at the University of Florida: Isomorphic Phase Transition and Cohesive Energy in Cs; Vanadium Non-Magnetic to Magnetic Transition with Lattice Size; and Soft X-Ray Emission Spectra of TiC and NbC.*†

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ABSTRACT

Self-consistent APW calculations have been performed to provide electron eigenvalues and wave functions for several systems, within the Xα approximation for the exchange and within the muffin-tin approximation for generating and utilizing the effective one-electron potential. This information has been used to calculate cohesive energies for metallic cesium and vanadium and to calculate the isomorphic phase transition of cesium. The formal magnetization of vanadium as a function of its lattice parameter has been examined and a magnetic transition found. Momentum matrix elements for titanium carbide and niobium carbide have been estimated to provide an approximate

expression for the energy dependence of the soft x-ray valence-band emission in terms of partial densities of states, allowing interpretation of the experimental data in terms of the calculated electronic properties.

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