Three Aspects of the Computation of Electronic Structures of
Metals at the University of Florida: Isomorphic Phase Transi-
tion and Cohesive Energy in Cs; Vanadium Non-Magnetic to Mag-
netic 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 transi-
tion 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.