

transition point. Either of the two magnetic moments calculated for $a = 7.0$ a.u. is obtained, depending on the magnitude of the initial assumed magnetic moment in the self-consistency iterations.

FIG. 5. Cohesive energy calculated for V, as a function of lattice parameter. The error bar indicates the experimental equilibrium lattice constant and cohesive energy, for comparison.

FIG. 6. Non-magnetic densities of states, showing the increase in the density of states at the Fermi energy which eventually gives rise to magnetic behavior as the lattice parameter is increased further.

FIG. 7. Magnetic densities of states for $a = 8.5$ a.u., for majority (α) and minority (β) spin, showing exchange shift between corresponding states with opposite spin, in the magnetic state.

FIG. 8. Soft X-ray emission spectra from TiC: C - K (solid curve), Ti - K (dotted), and Ti- $L_{II,III}$ (dashed) spectra, as reported in references [22], [21], and [23], respectively.

FIG. 9. Soft x-ray emission spectra from NbC: C - K, Nb - L_{III} , and Nb - $M_{IV,V}$, from reference [25].

FIG. 10. Decomposition of the Ti- $L_{II,III}$ emission spectrum from TiC into separate, proportional L_{II} and L_{III} components, separated by the energy splitting between the atomic L_{II} and L_{III} peaks.

FIG. 11. Experimental C-K emission (smooth curves) from TiC, according to Holliday [22] as reported by Ramqvist et al. [21], and C - $\ell = 1$ partial density of states. Dashed curve corresponds to an 0.6 eV adjustment in relative Fermi energies.

FIG. 12. Experimental Ti-K emission curves and calculated Ti- $\ell = 1$ partial density-of-states histogram for TiC. Dotted curve is from Nemnonov and Kolobova [26]. Solid is uncorrected and dashed is corrected data from Ramqvist, et al. [21]. Dot-dash curve is obtained from shifting dashed curve by 0.6 eV.

FIG. 13. Ti - L_{II} (from Fischer [23]) emission (smooth curves) and Ti- $\ell = 2$ curves for TiC. Result of 0.6 eV shift is shown as dashed curve.

FIG. 14. Comparison of C - $\ell = 1$ partial density of states (histogram) for NbC with the C-K emission (smooth curve) reported by Ramqvist, et al. [25].

FIG. 15. NbC Nb - L_{III} emission, from Ramqvist, et al. [25], compared with the Nb- $\ell = 2$ partial density of states.

FIG. 16. Partial Nb - $M_{IV,V}$ emission, from Holliday [25], and Nb - $\ell = 1$ partial density of states. Dashed curve shows correction for apparent spectrometer calibration error, reported by Ramqvist et al. [25]. An additional peak in the spectrum has now been observed [24], in good agreement with the partial-density-of-states peak at about -11 eV. Separation of the two Nb-M peaks shown is also the energy