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Evolution of the Spin Magnetic Moments and Atomic Valence of Vanadium in Vanadium doped Copper, Silver, and Gold Clusters.[1]
ARTHUR REBER, Department of Physics, Virginia Commonwealth University, WILLIAM BLADES, Department of Material Science and Enginieering, University of Virginia, SHIV KHANNA, Department of Physics, Virginia Commonwealth University — The atomic structures, bonding characteristics, spin magnetic moments, and stability of VCu_x^+, VAg_x^+, and VAu_x^+ (x = 3 - 14) clusters have been examined using density functional theory. Our studies indicate that the effective valence of vanadium is size-dependent and at small sizes some the valence electrons of vanadium are localized on vanadium while at larger sizes the $3d$ orbitals of the vanadium participate in metallic bonding eventually quenching the spin magnetic moment. The electronic stability of the clusters may be understood through a split-shell model that partitions the valence electrons in either a delocalized shell or localized on the vanadium atom. A molecular orbital analysis reveals that in planar clusters the delocalization of the 3d orbital of vanadium is enhanced when surrounded by gold due to enhanced *6s-5d* hybridization. Once the clusters become three-dimensional, this hybridization is reduced and copper most readily delocalizes the vanadium's valence electrons. By understanding these unique features, greater insight is offered into the role of a host materials electronic structure in determining the bonding characteristics and stability of localized spin magnetic moments in quantum confined systems.

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