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Spin Moments and Stability of VCun+ Clusters: The curious case of VCu_4^+, VCu_8^+, and VCu_{12}^+[1] WILLIAM BLADES, ARTHUR REBER, SHIV KHANNA, VCU, LUIS SOSA, PATRIZIA CALAMINICI, ANDREAS KOSTER, Civestav — The atomic structures, bonding characteristics, magnetic spin moments, and stability of VCu_n^+ clusters have been examined within density functional theory. Our studies show that at small sizes, the spin moments of the vanadium atom ($3d^3$ $4s^2$) due to 3d electrons are unquenched as the bonding is primarily through 4s electrons. As the cluster grows, the 3d orbitals of the vanadium atom start to participate in hybridized bonding with the copper atoms, resulting in a quenching of the magnetic moment. Upon closer examination of the electronic structures, we observe shell closure at VCu_5^+, VCu_7^+, and VCu_{14}^+. However, the observed abundances in the photofragmentation profile do not correspond to these shell closures and the subsequent electronic stability they provide. Instead, the enhanced abundances of VCu_4^+, VCu_8^+, and VCu_{12}^+ seen in the mass spectrum are justified through geometric means and a cluster growth mechanism is proposed. Through synergetic theoretical and experimental efforts, the unusual enhanced stability of VCu_4^+, VCu_8^+, VCu_{12}^+, and their magnetic properties are probed and explained.

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Shiv Khanna
Virginia Commonwealth University

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