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On the Structure and Stability of Cu_nV and Ag_nV Clusters: Insight from an ab-intio Density Functional Investigation

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The evolution of structures, bonding characteristics, stability and spin magnetic moment of neutral and catonic Cu_nV and Ag_nV clusters with n ranging from 1 to 15 have been investigated using a first-principle density functional theory approach by employing the deMon2k [1] program. Born-Oppenheimer molecular dynamics (BOMD) simulations were performed at different temperatures and different initial structures along these trajectories were taken for which successive geometry optimizations without symmetry constraint were performed. The obtained results are analyzed and discussed in comparison with the experimental mass spectra of Cu_nV^+ and Ag_nV^+ [2,3]. In this talk globally optimized Cu_nV^+ [4] clusters are compared with their Ag_nV^+ [5] counterparts in order to gain insight into the abundance pattern of the mass spectra. One of the objectives is to examine the evolution of the valence with size and how this change is reflected in the change in multiplicity of the clusters.

[1] See http://www.demon-software.com
[2] E. Janssens, S, Neukermans, H.M.T. Nguyen, M.T. Nguyen, P. Lievens, *Phys. Rev. Lett.* **94**, 113401 (2005)
[3] P. Lievens *et al.*, private communication
[4] V.M. Medel, A.C. Reber, V. Chauhan, P. Sen, A.M. Köster, P. Calaminici, S.N. Khanna, *J. Am. Chem. Soc.* **136**, 8229 (2014).
[5] L. López Sosa *et al.*, in preparation