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Crystal Field Splitting and Stabilization of CuMgx- Clusters VICTOR M. MEDEL, J. ULISES REVELES, A.C. REBER, M.C. QIAN, S.N. KHANNA, Virginia Commonwealth University, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — The electronic states in clusters group into shells much in the same way as in atoms. Clusters with filled electronic shells exhibit enhanced stability as manifested through observed magic numbers in metal clusters. An important issue is if stable species can be attained at sub-shell fillings. In this work we have carried out first principles electronic structure calculations on CuAl_x^- and CuMg_x^- clusters to demonstrate this intriguing effect. It is shown that the ionic cores in the clusters can order to generate internal electric fields that lead to splitting of the supershells, much in the same way as the crystal field splitting of atomic states in crystals. The studies offer a new approach to forming magic species though control of the composition and the arrangement of atoms. The talk will highlight these effects and how they can be seen in experiments.

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