Abstract Submitted
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**Stability and Shell Magnetism in Transition Metal Doped Calcium clusters**[1] VICTOR M. MEDEL-JUAREZ, J. ULISES REVELES, S.N. KHANNA, Virginia Commonwealth University, V. CHAUHAN, P. SEN, Harrish-Chandra Research Institute, Chhatnag Road Jhunsi, Allahabad 211019, India — Clusters of many metallic elements are known to exhibit enhanced stability at valence electron counts 2, 8, 18, 20, 34, 40... that can be understood within a simple spherical confined nearly free electron gas model. In this work we show a magnetic species whose stability is rationalized on a modification of the above shell sequence through deformations of the spherical geometry and through enhanced exchange splitting of the electronic shells via impurity atoms with large atomic orbital exchange splitting. Through first principles theoretical studies of the electronic structure and stability of $TMCa_8$ (TM= Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Zn) clusters we identify a stable magnetic $FeCa_8$ cluster of 24 valence electrons distributed into a closed 1S2 1P6 1D10 2S2 shell sequence of 20 paired electrons and with 4 electrons occupying the majority $2D_{xy}2D^{22}_{x-y}$, $2D_{xz}$ and $2D_{yz}$ levels while the unfilled $2D^2_z$ level is separated by a large energy gap of 0.61 eV arising from atomic deformation.

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