Abstract Submitted
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Chromium Oxide Clusters as Building Blocks to Nanoscale Materials[1] S.N. KHANNA, N.O. JONES, Physics Department, Virginia Commonwealth University, Richmond, Virginia 23284, D.E. BERGERON, A.W. CASTLEMAN, Departments of Chemistry and Physics, 152 Davey Laboratory,The Pennsylvania State University, University Park, PA 16802 — It is shown that by varying the formation conditions, two distinct families of stable chromium oxide nanoparticles can be generated, each with unique electronic and magnetic properties. The clusters are found to demonstrate remarkable stability, acting as building blocks and providing the framework to form extended structures. By use of gradient corrected density-functional theory and mass spectra data, we demonstrate that different classes of stable oxygen-passivated chromium oxide clusters have class-specific electric and magnetic properties. More specifically, irrespective of cluster size, the Cr_nO_{2n+2} cages are ferromagnetic, and the saturated rings of Cr_nO_{3n} are nonmagnetic. The rings are characterized by high electron affinities in addition to their stability and an investigation into the formation of ionic molecules upon combination with alkali atoms is addressed.

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