

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A Theoretical Study of Structural, Electronic and Vibrational Properties of Small Fluoride Clusters KEVIN WATERS, Department of Physics, Michigan Technological University, RATNESH PANDEY, Nanotechnology Application Centre, University of Allahabad, SANDEEP NIGAM, Chemistry Division, Bhabha Atomic Research Centre, HAIYING HE, Department of Physics and Astronomy, Valparaiso University, SUBHASH PINGLE, Department of Chemistry, University of Pune, AVINASH PANDEY, Nanotechnology Application Centre, University of Allahabad, RAVINDRA PANDEY, Department of Physics, Michigan Technological University — Alkaline earth metal fluorides are an interesting family of ionic crystals having a wide range of applications in solid state lasers, luminescence, scintillators, to name just a few. In this work, small stoichiometric clusters of $(MF_2)_n$ ($M = \text{Mg, Ca, Sr, Ba}$, $n=1-6$) were studied for structural, vibrational and electronic properties using first-principles methods based on density functional theory. A clear trend of structural and electronic structure evolution was found for all the alkaline earth metal fluorides when the cluster size n increases from 1 to 6. Our study reveals that these fluoride clusters mimic the bulk-like behavior at the very small size. Among the four series of metal fluorides, however, $(\text{MgF}_2)_n$ clusters stands out to be different in its preference of equilibrium structures owing to the much smaller ionic radius of Mg and the higher degree of covalency in the Mg-F bonding. The calculated binding energy, highest stretching frequency, ionization potential, and HOMO-LUMO gap decrease from MgF_2 to BaF_2 for the same cluster size. These variations are explained in terms of the change in the ionic radius and the basicity of the metal ions.

Kevin Waters
Department of Physics, Michigan Technological University

Date submitted: 14 Nov 2013

Electronic form version 1.4