Geometric and electronic structures of halogen (M)-doped aluminium clusters: MAln(M=F, Cl; n=3-15)

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Abstract

The equilibrium geometries, stabilities, and electronic properties of MAln(M=F, Cl; n=3-15) are calculated by employing CALYPSO global search technique combined with B3LYP scheme. Optimized geometries for FAln and ClAln clusters displayed that the rule of structural evolution is attaching type, and in the end to the cage-like pattern with Al atom located inside Aln clusters (n=12-15). The analysis of stabilities shown that the FAl7 and ClAl7 clusters are the magic numbers with good chemical stabilities. The analysis of internal charge transfer shown that F or Cl atom is an electronic acceptor and strong sp hybridization exists in the F or Cl atom. Finally, the chemical hardness and polarizabilities are discussed.

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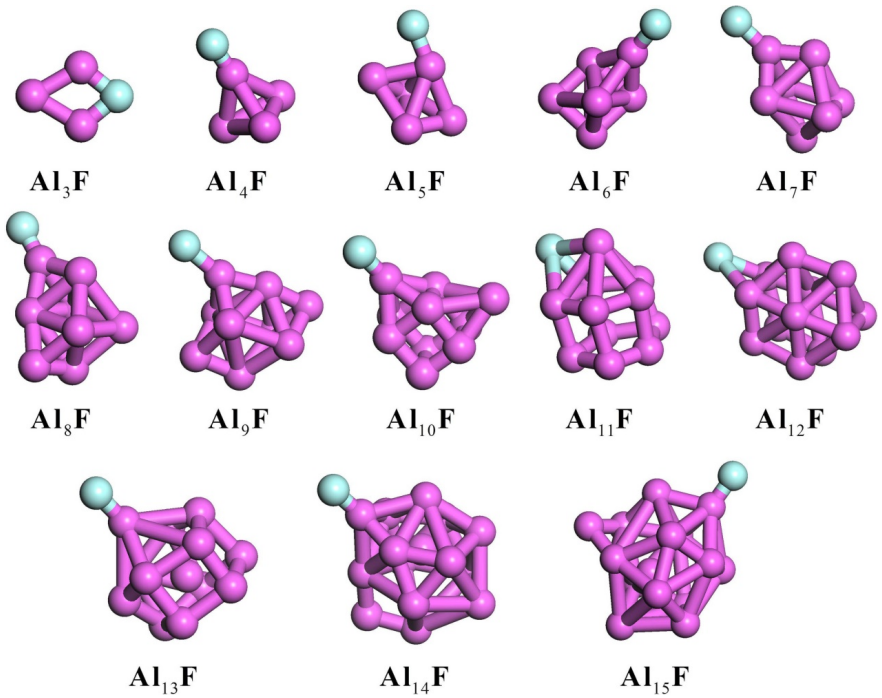

Figure 1. The ground state structures of Al_n F(n =3-15) clusters. Purple and azure balls represent Al and F atoms, respectively.

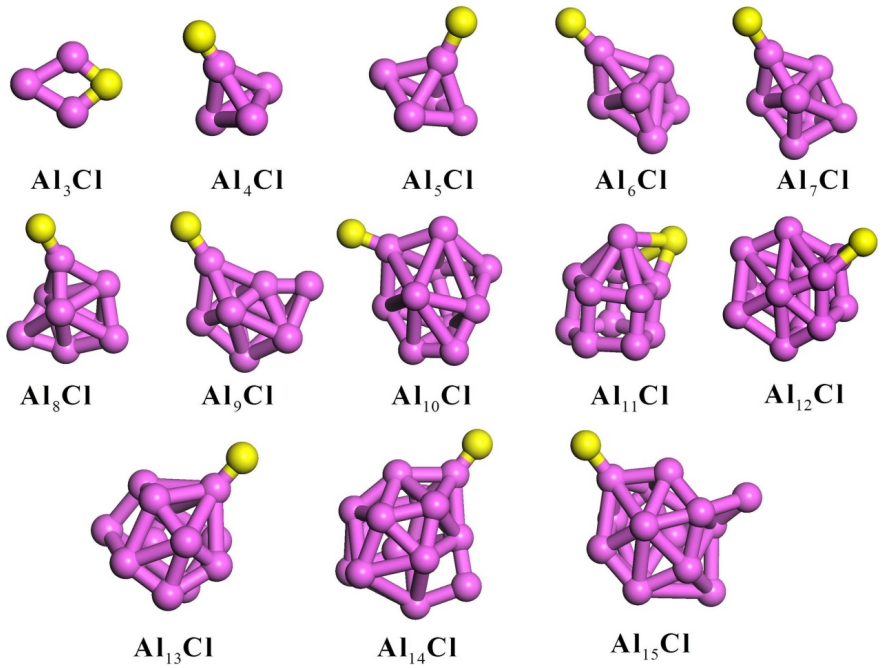

Figure 2. The ground state structures of Al_n Cl(n =3-15) clusters. Purple and yellow balls represent Al and Cl atoms, respectively.

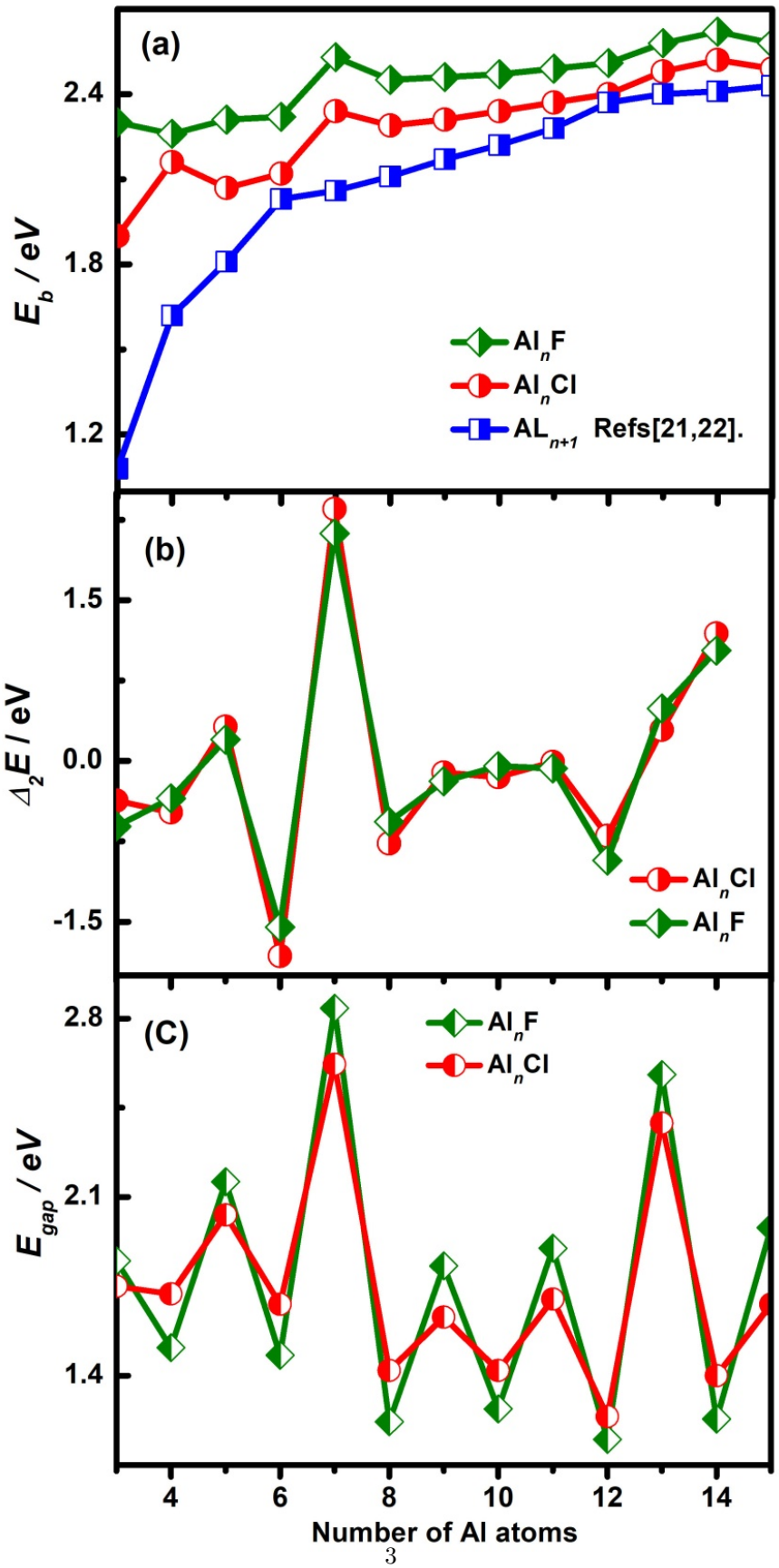

Figure 3. The size dependence of the averaged binding energy E_b (a), second-order difference energy $\Delta_2 E$ (b), and HOMO-LUMO energy gap E_{gap} (c) of ground state MAl_n (X=F, Cl; n =3-15) clusters

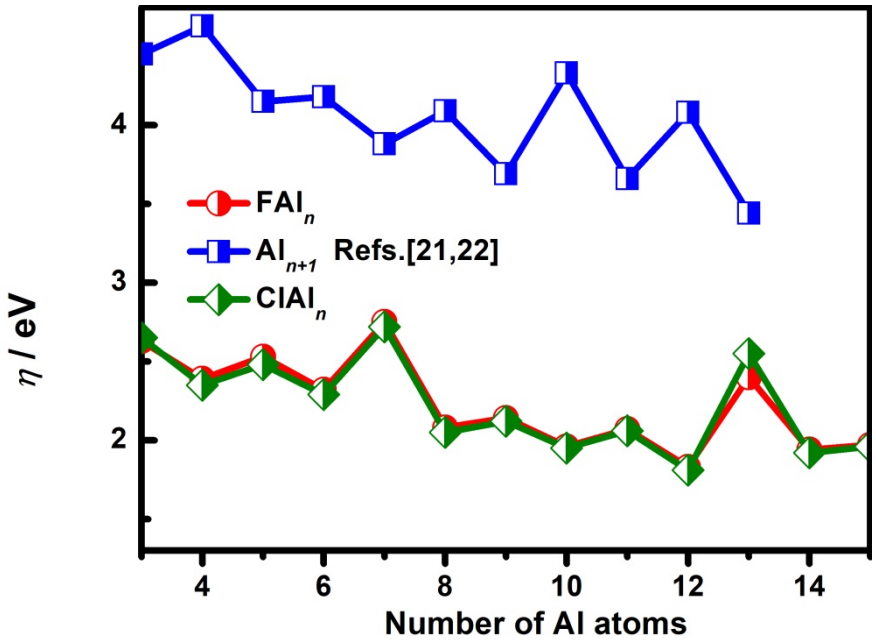

Figure 4. The chemical hardness of ground state MAl_n (X=F, Cl; n =3-15) clusters.

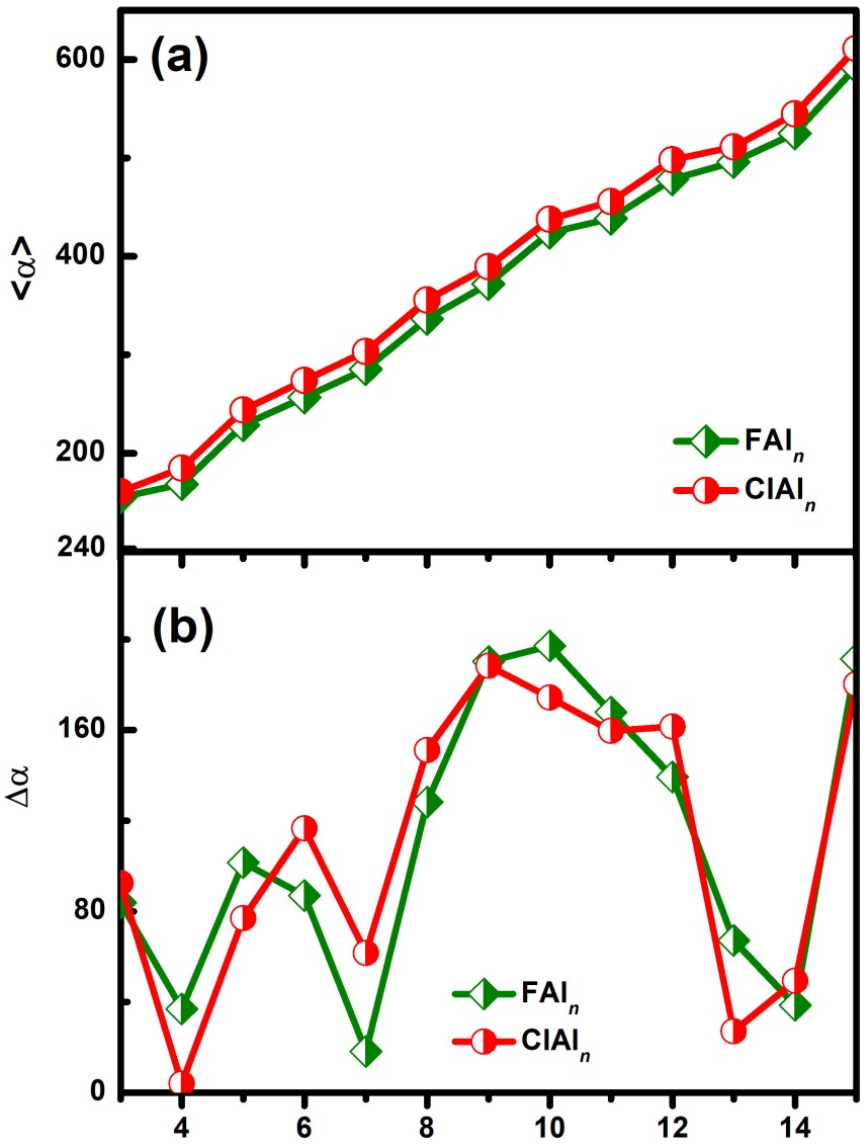

Figure 5. The static mean polarizabilities (<α>)(a), and polarizability anisotropies (Δα)(b) of ground state MAl_n (X=F, Cl; n =3-15) clusters.