Theoretical Analysis of the Electronic Properties of the Endohedral Clusters M@Al_{12} (M= B, Al, Si, N, P) and their ions

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It is well established that endohedral anion clusters M@Al12 (M= B, Al, Si, N, P) have high stable icosahedral structures with a HOMO-LUMO gap comparable to C60 and Au20. However, when ionized, they present a vibronic instability tending to break their symmetry. In this work we present an analysis, based on an all-electron full relativisic DFT calculation, showing that trough the ionization process ending with 39 and 41 electrons, these anion clusters suffer a Jahn-Teller symmetry breaking. The original Ih structure symmetry of the anion clusters (with 40 electrons), is lowered to D2h for B and D3d for Al, Si, N, and P in the 39 electrons case; and D5d for the 41 electrons structure, except for N. We present the results for the corresponding density of states, vertical detachment energies and vertical ionization potentials. We discuss our results within the framework of the superatom model.