SYMMETRY-PRESERVED SUPERATOMIC ORBITALS IN I_h ALUMINUM CLUSTERS: SEPARATING ELECTRON COUNT AND NUCLEAR GEOMETRY VIA THE SHELL POTENTIAL

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Understanding whether superatomic electronic structures are governed primarily by electron count [1] or by nuclear geometry remains a fundamental question in cluster chemistry. In this study, we disentangle these two effects by directly comparing I_h-symmetric Al_{13} and Al_{12} clusters under an identical geometric framework. While Al_{13} possesses 39 valence electrons—close to the jellium magic number of 40—and Al_{12} contains 36 electrons, symmetry analysis reveals that the sum of irreducible representations of the valence-occupied superatomic orbitals is conserved in both systems.

This invariance demonstrates that the fundamental orbital framework is dictated predominantly by the I_h-symmetric Al_{12} shell rather than by electron count or the mere presence of the central atom. The core Al atom instead acts as a strong central potential that modifies energy levels and spatial distributions without reconstructing the orbital skeleton.

To formalize this separation, we introduce the SHELL (Spherical Hydrogen-like Effective Localized Layer) Potential (**Fig. 1**), an analytical mean-field model that explicitly decomposes the effective potential into shell-derived and core-derived contributions. Unlike the conventional jellium picture [2] assuming a uniform positive background, the SHELL Potential represents the nuclear charge as a radially localized geometric layer, directly incorporating structural symmetry into the confining field.

This framework provides a physically transparent description of symmetry-preserved superatomic orbitals and offers a transferable perspective for understanding and designing high-symmetry superatomic systems beyond Al_{13}.

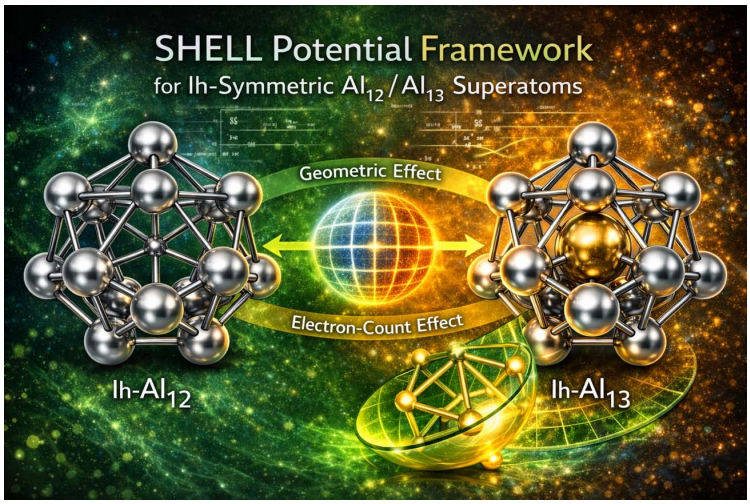

Fig. 1. SHELL Potential framework for I_h aluminum superatoms. The geometric Al_{12} shell preserves the symmetry and degeneracy pattern of superatomic orbitals, while the central Al atom primarily modulates the energy via a core-derived potential. The effective mean field is separated into shell and core contributions.

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[1] Z. Luo and A. W. Castleman, *Acc. Chem. Res.*, 2014, **47**, 2931-2940.

[2] K. Clemenger, *Phys. Rev. B*, 1985, **32**, 1359-1362.