

Supplementary information of:
Principles of isomer stability in small clusters

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In the following we show two additional analysis concerning the redistribution of the electronic charge density for selected Na and Mg clusters together with various figures from the main publication augmented by the data used to make the figure plus selected structural and electronic properties.

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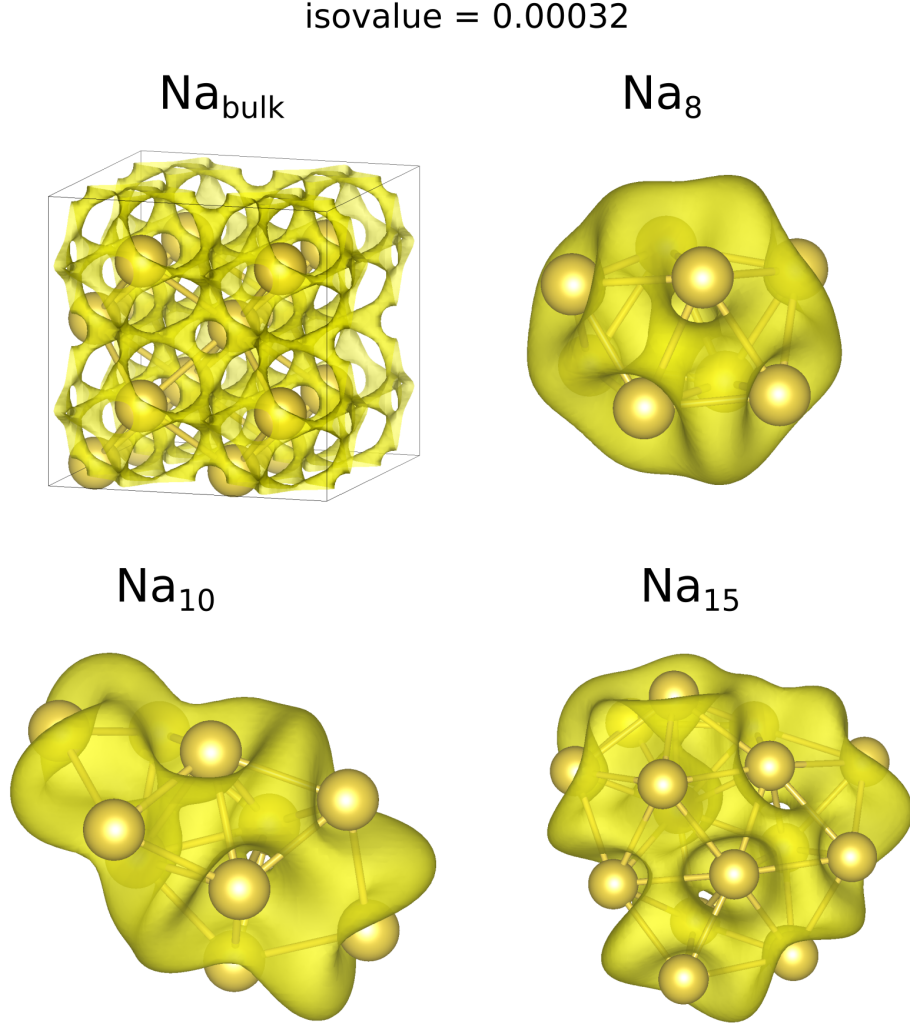


FIG. S1. Difference between the selfconsistent DFT charge density and the sum of the atomic charge densities of spherically symmetrized atoms. For each iso-value only the positive part is shown which illustrates the flow of the electronic charge density when the structure is formed out of individual atoms. All representations refer to an isovalue of 0.00032. Top row shows the charge difference for bulk Na and the global minimum of the Na_8 cluster. Bottom panels in the second row show the charge difference for the global minima of the Na_{10} and Na_{15} clusters. For large identical iso-charge values, the volume included by the iso-surface is always substantially larger in the case of the clusters compared to the solid. Since these regions of high charge densities are in between neighboring atoms, the bonds are contracted in the cluster compared to the solid.

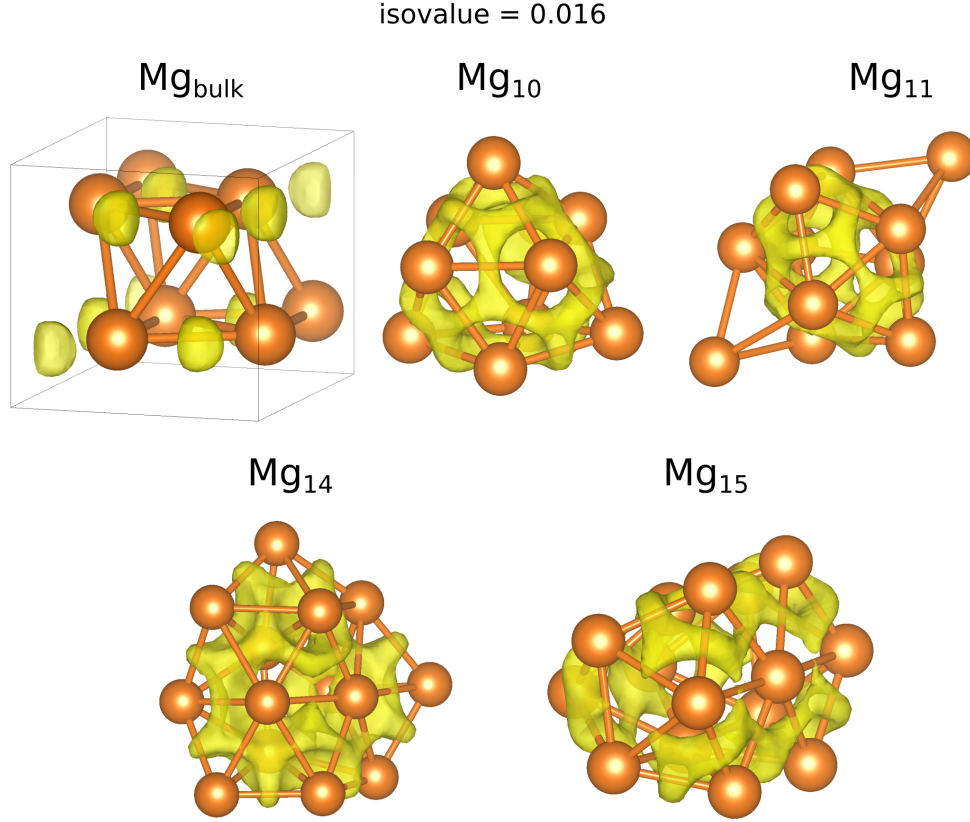


FIG. S2. Difference between the selfconsistent DFT charge density and the sum of the atomic charge densities of spherically symmetrized atoms. For each iso-value only the positive part is shown which illustrates the flow of the electronic charge density when the structure is formed out of individual atoms. All representations refer to an isovalue of 0.016. Top row shows the charge difference for bulk Mg and the global minima of the Mg_{10} and Mg_{11} clusters. Bottom panels in the second row show the charge difference for the global minima of the Mg_{14} and Mg_{15} clusters. For large identical iso-charge values, the volume included by the iso-surface is always substantially larger in the case of the clusters compared to the solid. Since these regions of high charge densities are in between neighboring atoms, the bonds are contracted in the cluster compared to the solid.

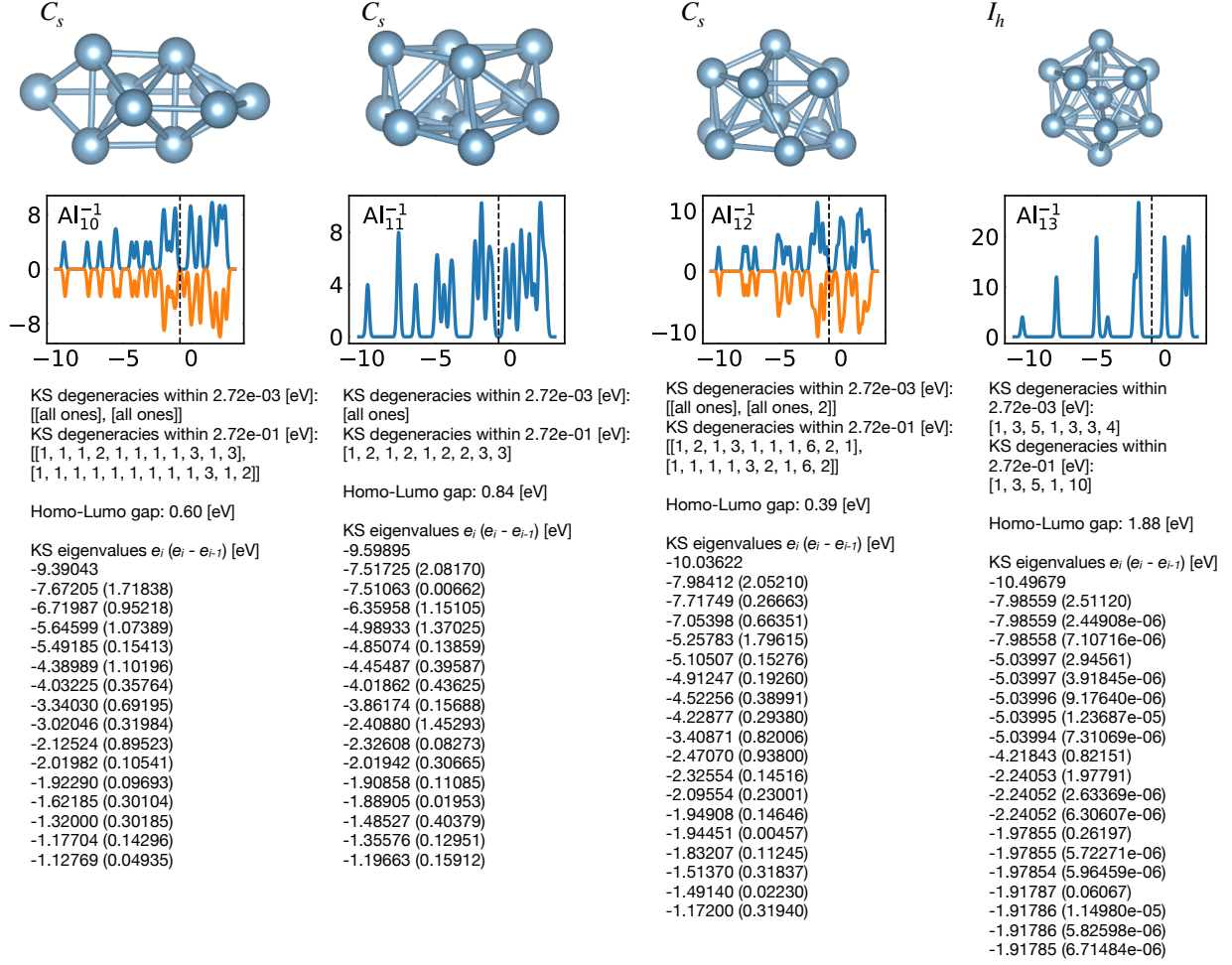


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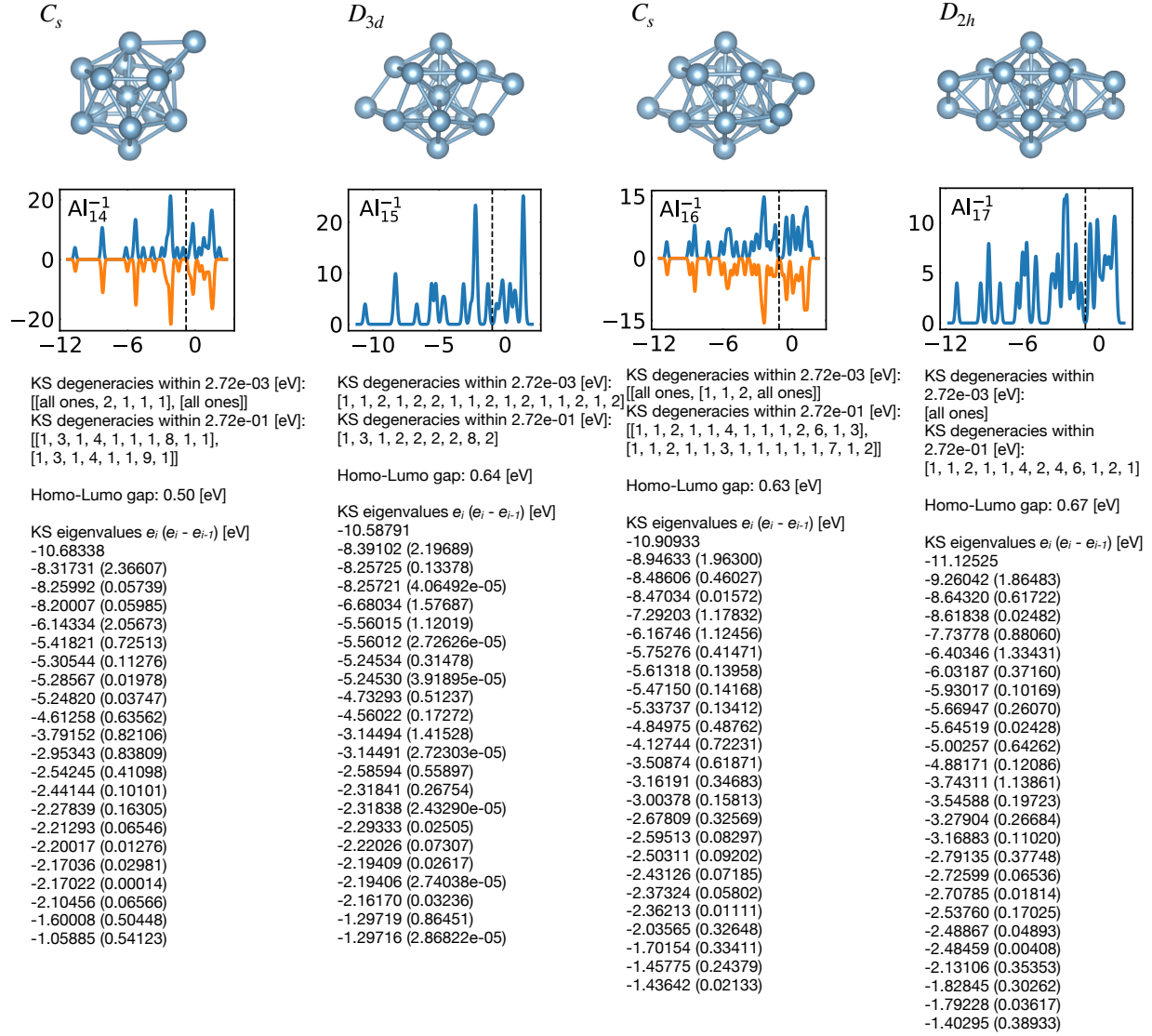


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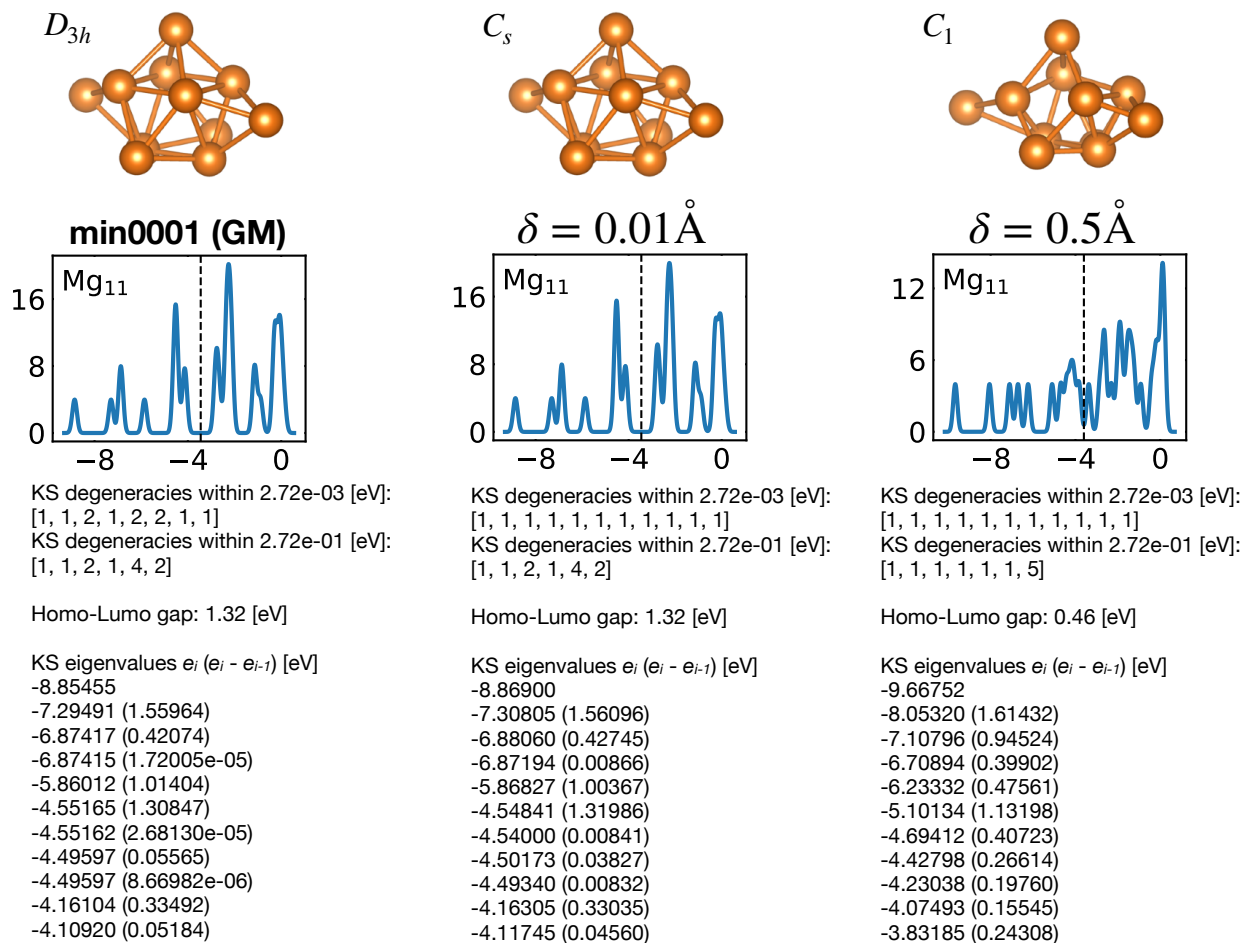


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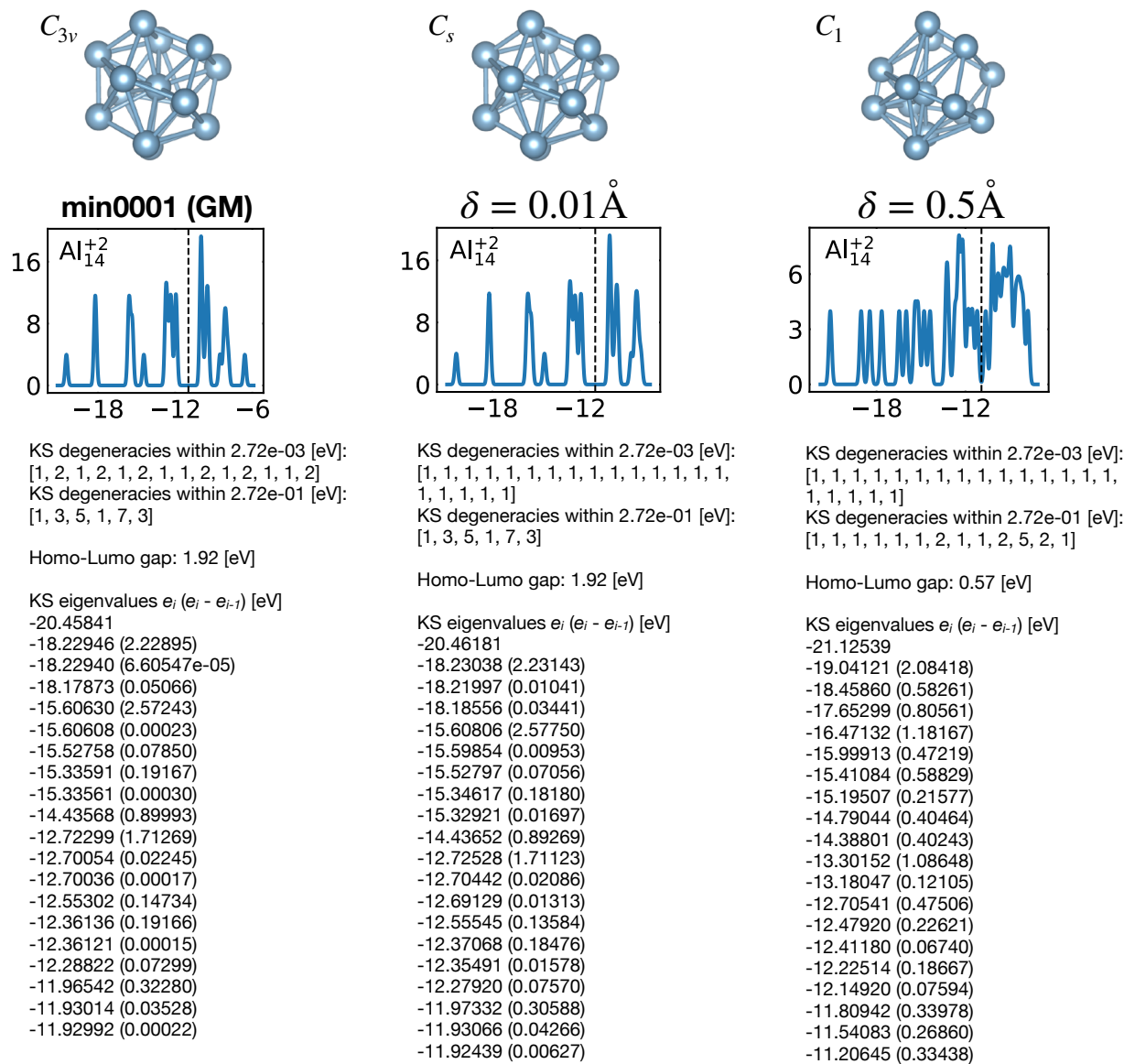


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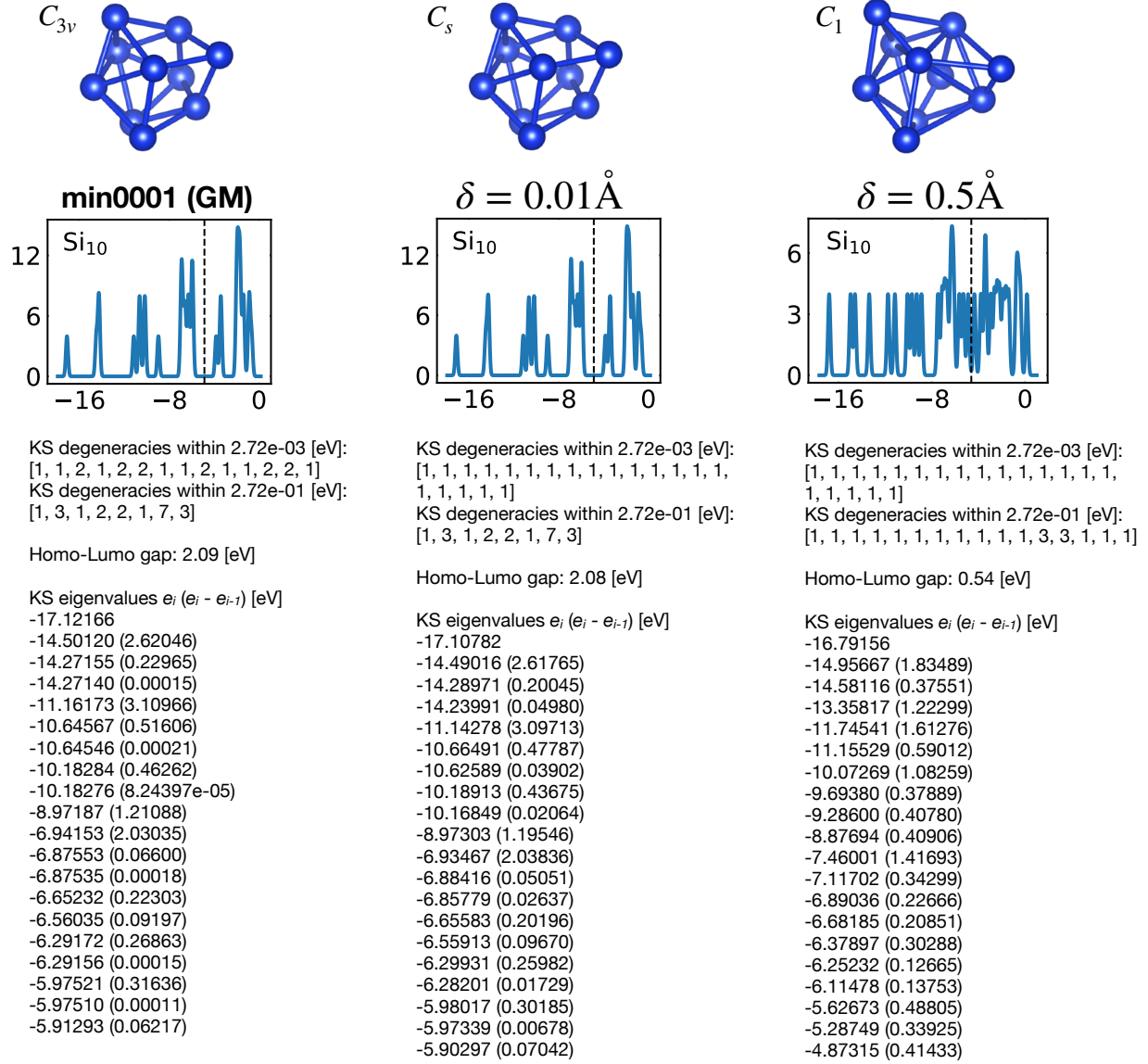


FIG. S4. Lifting of the KS eigenvalue degeneracies by random atomic displacements away from the global minima. The effect for two different displacement amplitudes δ is shown, $\delta = 0.01$ and $0.5 \text{ \AA}$.

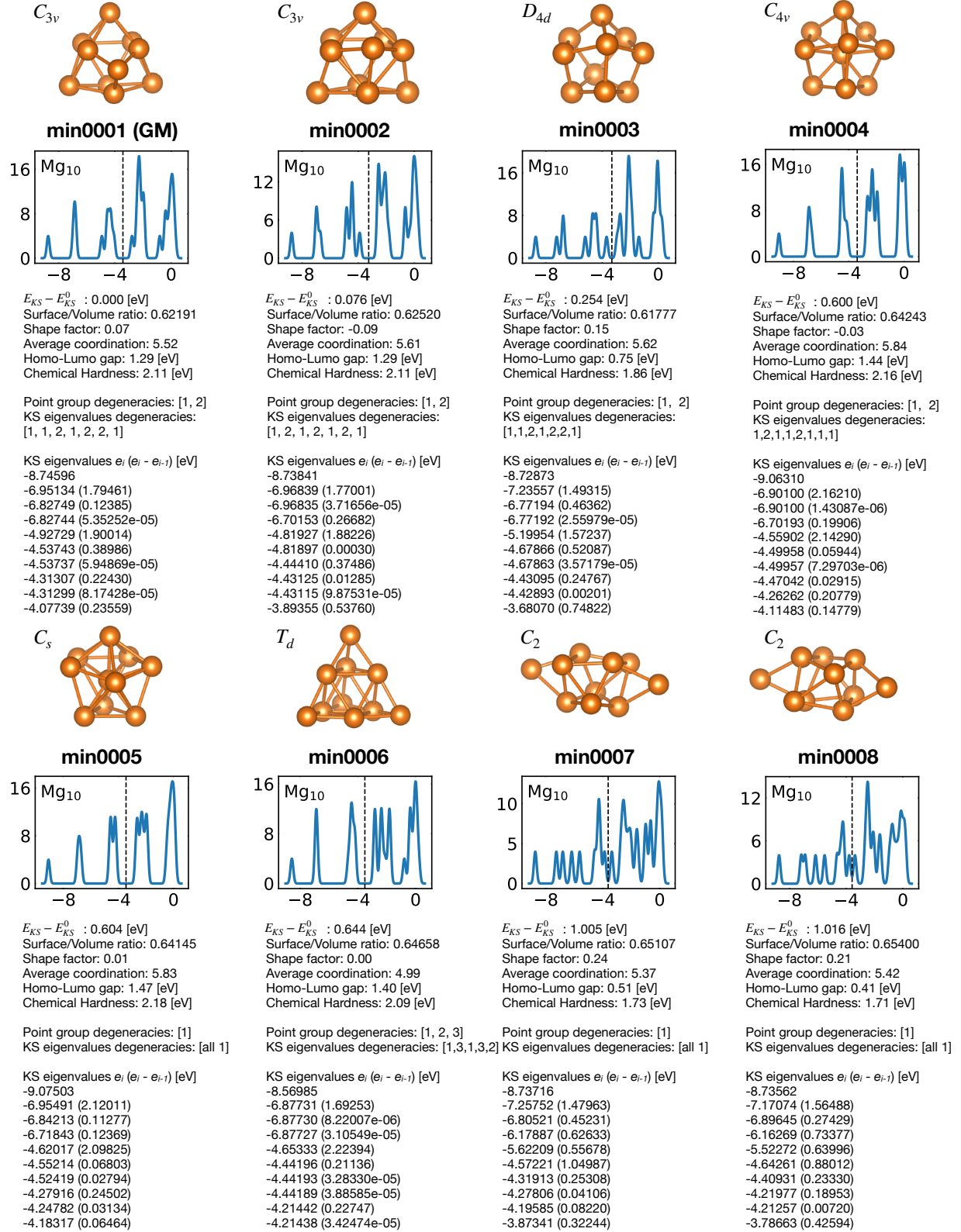


FIG. S5. Structural and electronic properties of the first eight low-lying minima for the Mg₁₀ cluster.

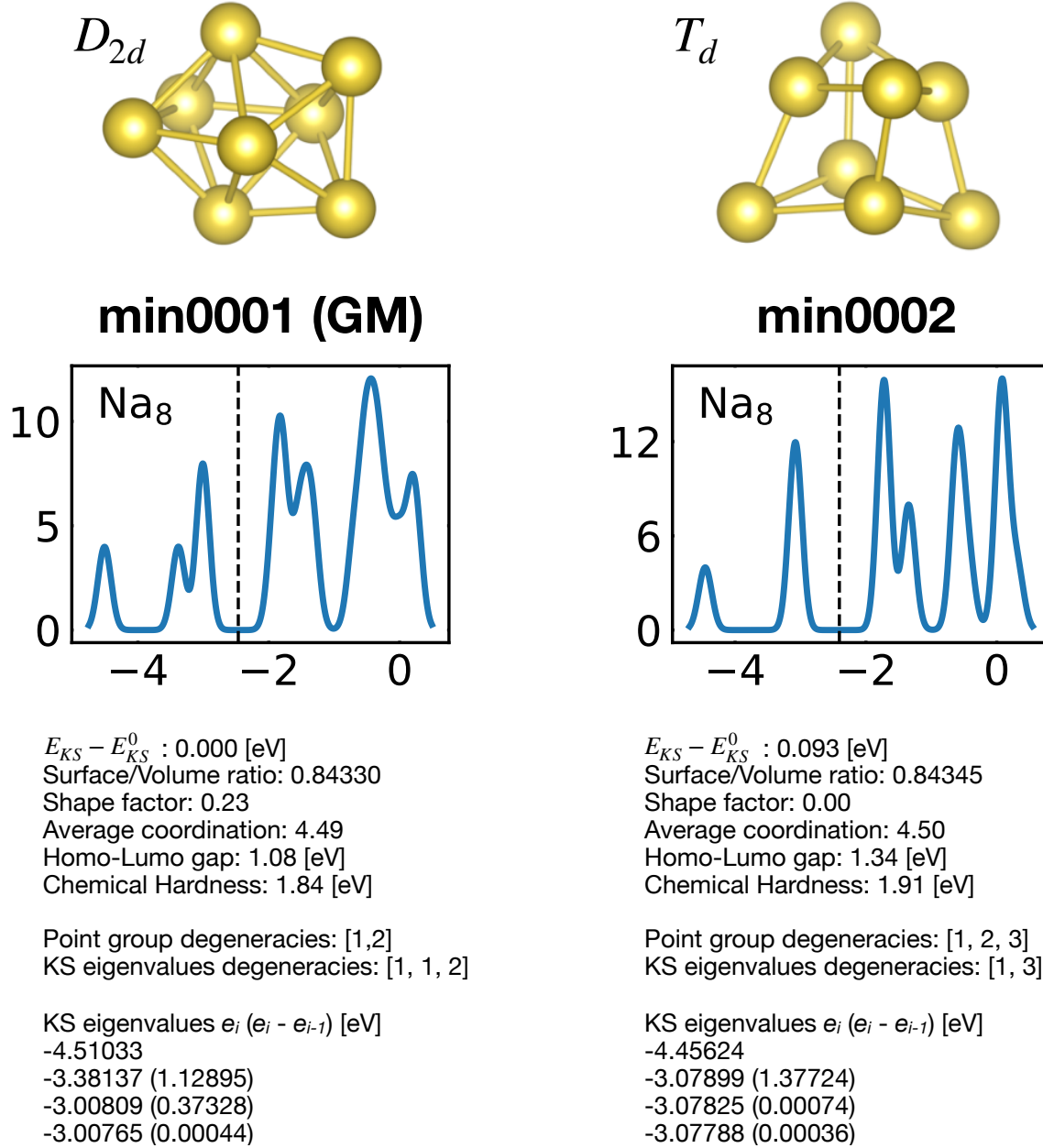


FIG. S7. Structural and electronic properties of the first two low-lying minima for the Na₈ cluster. The two structures are completely unrelated and the degeneracy of the KS eigenvalues in the ground state is accidental and not caused by symmetry.

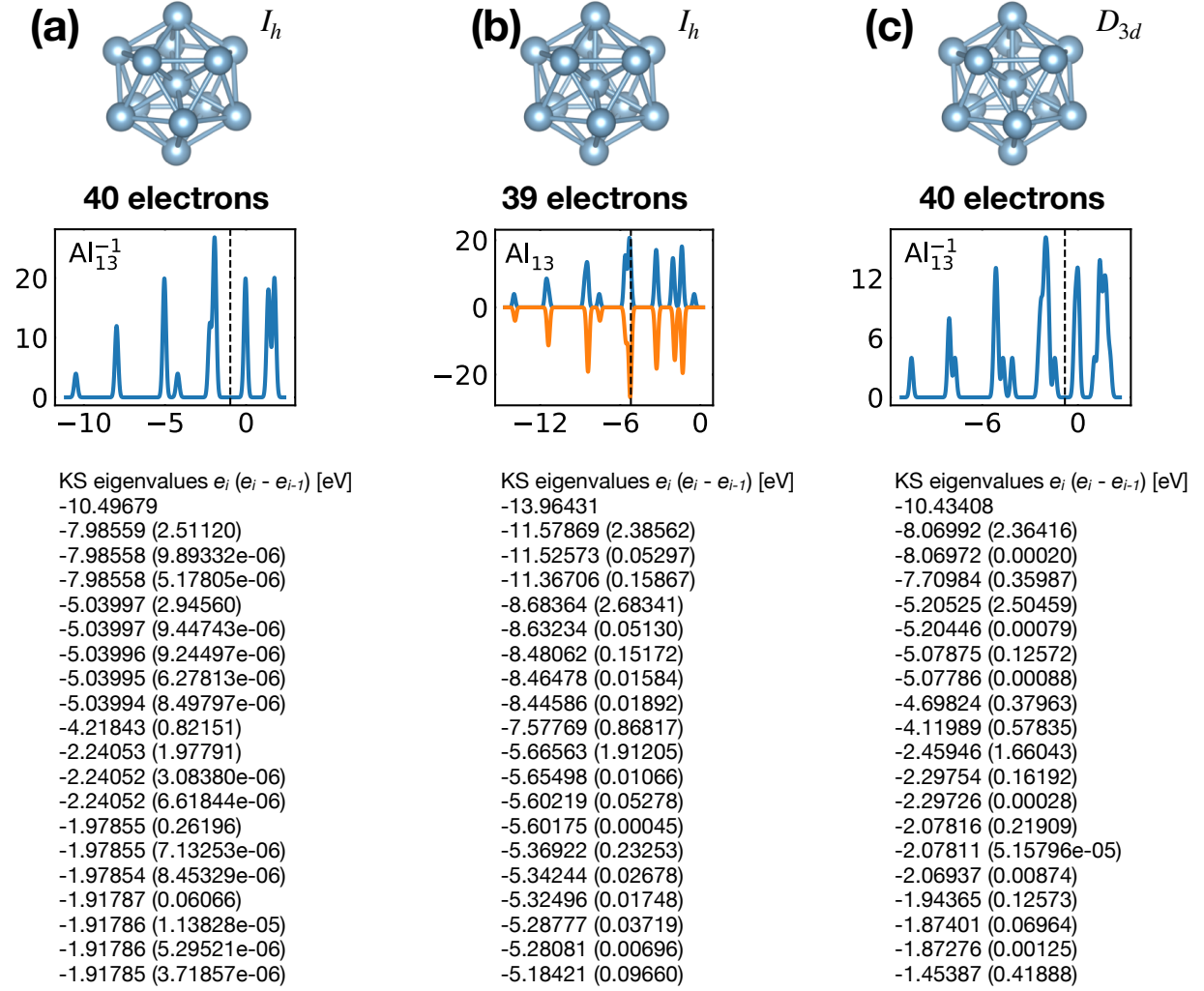


FIG. S8. Density of states of 40 (a) and 39 (b) valence electrons, distributed over a perfect icosahedron with point group I_h . This structure is the GM of Al_{13}^{-1} and has point group degeneracies [1, 3, 4, 5]. (c) shows the DoS of 40 electrons distributed over the slightly distorted icosahedron D_{3d} GM of Al_{13} which has point group degeneracies [1, 2].