

On the Search of Small Cu-Ru Atomically Precise Superatoms. Cu₁₀Ru Cluster as a Stable 18-ve Endohedral Structure

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Abstract

Atomically precise metallic clusters behaving as superatoms, are relevant building blocks towards new materials under the bottom-up approach. Here we discussed the plausible formation of the Cu₁₀Ru cluster as a superatomic specie accounted its 1S₂ 1P₆ 1D₁₀ shell order, with the aim of identification of particular clusters with enhanced stability. By stochastic structure search on Cu₁₀Ru clusters, we found six low-lying cluster isomers with ΔE values from 0.0 to 4.7 kcal[?]/mol above the ground state denoting an endohedral motif with the Ru dopant inside the Cu₁₀ cage, as the favored structures. By using molecular dynamics simulations we found a clear trend of encapsulation of the Ru atom at low temperatures, quantified by the Cu-Ru bonding distances during the annealing procedure. The 17-ve counterpart, Cu₉Ru shows a large electron affinity, owing to the trend to achieve a electronic shell closing as a new superhalogen species. These results are useful for further rationalization and design of novel superatoms expanding the libraries of endohedral clusters.

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