

Abstract Submitted
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Geometrical and electronic properties of sodium, copper, and silver clusters: A comparative study¹ MINGLI YANG, KOBLAR A. JACKSON, Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859, JULIUS JELLINEK, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 — The structures of sodium, copper, and silver clusters with up to 20 atoms are investigated using density functional theory computations. Utilizing an extensive unbiased search procedure, we first find a large number of low-energy isomers of Cu clusters. The structures of these isomers are then reoptimized for Na and Ag clusters. We find a strong propensity to form similar conformations for clusters of these three elements. In most cases their energetically preferred forms have the same packing. As the cluster size increases, it changes from planar (less than 7 atoms) to layered (7 to 16 atoms) and eventually to compact (17 to 20 atoms). The similarities and differences between the clusters of the three elements will also be characterized in terms of their electronic properties such as ionization potential, HOMO-LUMO gap, dipole moment, and polarizability.

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