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Structural, electronic and magnetic properties of 22-, 35-and 55-atom core-shell Au-Cu nanoclusters
(2013) *Molecular Simulation*, 39 (6), pp. 505-512. Cited 3 times.

Abstract
Compared to monometallic clusters, bimetallic nanoclusters combine the distinctive properties of varied materials and thus exhibit a broader range of the degrees of freedom due to the presence of two different metals. This affords greater opportunity to control their properties by modifying composition as well as size. In this work, we investigated magnetic and electronic properties for Au-Cu bimetallic core-shell structures using the first-principle calculations based on the density functional theory. Our work indicated that the Au-Cu core-shell can have a half-metal property through chemical composition modification. Half-metallic ferromagnets attract increasing research interest as potential materials for spintronic device applications. Au20Cu2 and Au32Cu6 clusters are half-metallic ferromagnets with large half-metallic gaps. © 2013 Copyright Taylor and Francis Group, LLC.

2-s2.0-84876297913
Document Type: Article
Publication Stage: Final
Source: Scopus