Natural arrangement of AgCu bimetallic nanostructures through oleylamine reduction

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Abstract
Noble-metal-based catalysts are the most used nanomaterials to carry out electrochemical reactions, which are commonly applied in fuel cells. This kind of catalyst is expensive and it is worth mentioning that noble metals are scarce. So, nanocatalysts based on cheaper metals, such as Ag and Cu, are highly desired. Here, we report the natural arrangement of different AgxCuy nanostructures through oleylamine reduction. Firstly, an experimental study was carried out in order to study the crystallographic structure, size, and shape of each synthesized nanostructure. The samples were fully characterized via powder X-ray diffraction, while scanning-transmission electron microscopy with a high-angle annular dark-field (HAADF) was applied to investigate the morphological features. Interestingly, the HAADF images of the AgCu NPs mostly show a Janus-type configuration, instead of a core-shell architecture, which is the most stable atomic arrangement. Given this, we subsequently performed classical molecular dynamics simulations under the NVT canonical ensemble to further deepen our study. The theoretical results pointed out that the nanostructure with a core-shell morphology is the one with the lowest energy. However, it also indicates an energy decrease in the Janus configuration, as long as the NP size increases. Therefore, for nanostructures with a large number of atoms, this could lead to a strong competition between Janus and core-shell arrangement. Finally, considering the AgCu NP size, it is worth noting that the theoretical data supports the experimental results, making these systems interesting not only because of their properties but also due to the relatively easy synthesis procedure.

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