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Structural stability of some gold (Au) and silver (Ag) nanoparticles

The classical molecular dynamics is used to study Au and Ag nanoparticles focusing mainly on their structural stability. The structures were modelled at various temperatures in an NVT Evans ensemble. As such, the many-body Sutton-Chen potential was initiated to describe the interactions between atoms in both nanoparticles. Variation of total energy with temperature was investigated for both Au and Ag nanoparticles; in the process, entropy was calculated. Radial distribution functions were utilised to predict the most probable Au and Ag nanoparticle structures. To probe the mobility of Au and Ag atoms in their systems, the mean square displacements (MSD) were plotted, in which the diffusion constants were calculated to be 0.58 Å2/ ps for Au and 1.87 Å2/ ps for Ag atoms.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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