Development of a Neural Network Potential to reproduce the potential energy landscape of gold AuN (N=10-120) anionic, cationic and neutral nanoclusters.

Investigadores:

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Idioma Sin definir

Descripción:

Proyecto asignado a través de la Red Española de Supercomputación (RES [2]).

First principles calculations are the standard approach to study nanostructures, which are based on the fundamental laws of quantum mechanics. There are several situations however in which these calculations are not feasible, for instance in large systems containing thousands of atoms, or when exploring the completeness of the energy potential landscape. Thus, other approaches emerge such as the interatomic potentials, or the novel Neural Network Potentials. Based on the Machine Learning technique, these combine the speed of empirical potentials while being substantially more accurate. We have developed a Neural Network Potential for nanostructures, and we aim to apply this scheme to gold nanoclusters, a system arduous to study by ab-initio calculations and challenging to depict through empirical potentials due to its complexity.

URL del envío:https://www.cenits.es/proyectos/development-neural-network-potential-reproduce-potential-energy-landscape-gold-aun-n10-120

Enlaces

[1] https://www.uva.es/ [2] https://www.res.es/