Funded by the European Union
cost EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY
4TH GENERAL MEETING OF COST ACTION CA21101 "COSY"
COSY COST ACTION
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES
CSIC

Gaussian Approximation Potentials for Adsorbate-Functionalized Pt–Cu Nanoparticles

Ilker Demiroglu[1]*

[1]*Eskisehir Technical University, Turkey*

Bimetallic Pt–Cu nanoparticles are attractive catalysts for oxidation and hydrogenation reactions due to their tunable electronic structure, reduced noble metal content, and enhanced resistance to surface poisoning. However, first-principles modeling of realistic nanoparticle sizes and morphologies remains computationally demanding. Here, we develop high-fidelity Gaussian Approximation Potential (GAP) models for Pt–Cu nanoparticles functionalized with single O_2 and CO molecules, enabling near–DFT-accurate simulations at a fraction of the computational cost. The training dataset was generated from ab initio molecular dynamics trajectories spanning temperatures from 300 to 1000 K and includes multiple particle sizes (38–260 atoms) and morphologies, such as pure, core–shell, Janus, and ordered alloy structures. The resulting GAP models reproduce DFT reference energies and forces with high accuracy, achieving root-mean-square errors below 0.4 meV atom^{-1} for energies and 70 meV Å^{-1} for forces, while remaining transferable across different structural motifs. Large-scale molecular dynamics simulations reveal that alloying Pt with Cu significantly improves thermal and mechanical stability. In particular, core–shell and Janus nanoparticles maintain ordered atomic coordination up to 1000 K, whereas monometallic counterparts exhibit increased surface disorder. Radial distribution function analysis confirms the persistence of short-range order under elevated temperatures and adsorbate presence. These results demonstrate that machine-learning-based interatomic potentials provide a robust and efficient framework for investigating adsorption-driven restructuring, morphology evolution, and thermal stability in bimetallic nanoparticles. The developed GAP models bridge the gap between quantum-mechanical accuracy and realistic length and time scales, offering valuable insights into composition–structure–stability relationships and supporting the rational design of cost-effective Pt–Cu catalysts for energy and environmental applications.