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DFT study of the structure, chemical ordering and molecular adsorption of Pd-Ir nanoalloys

Challenges

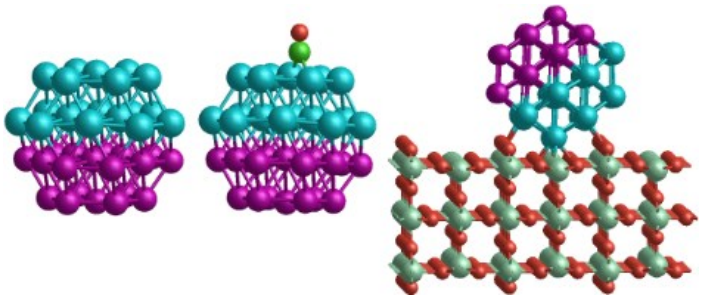
To explore the structural stability of nanoalloys with different chemical orderings and the preferred adsorption sites of molecules on metal nanoalloys.

Background

Metal nanoclusters are of interest as catalysts due to their high surface-volume ratio and high proportion of low-coordinated active sites. The (geometric and electronic) structures of metal nanoalloys are crucial to the understanding of their catalytic performances because the activity and selectivity are closely associated with structure. The catalytic performance also depends on composition, surface segregation and chemical ordering, and these characteristics of alloyed NPs can be controlled to tune their optical, electrical, and catalytic properties. The surface sites and the bonding of adsorbates under reaction conditions can also affect the surface structure and change the activity and the selectivity of nanocatalysts.

Results

In our research, all calculations are performed using the DFT method, as implemented in the Vienna ab initio Simulation Package (VASP) code on BlueBear high performance computer. The structural stability of 38-atom and 79-atom truncated octahedral (TO) Pd-Ir nanoalloys are investigated. Then the adsorption properties and preferred adsorption sites of CO on 38-atom Pd-Ir nanoalloys are considered. All calculated clusters are locally geometrical optimized at the DFT level, where all cluster atoms, are relaxed until the forces on the atoms are lower than 0.01 eV $Å^{-1}$. The BlueBear computer allows high-class computational facilities to perform these calculations. Our results of CO adsorption on Pd-Ir nanoalloys show the consistency with previous computational and experimental studies of CO on Pd and Ir surfaces. The study provides a valuable theoretical insight into catalytically active Pd-Ir nanoalloys.



The stability and chemical ordering properties of free, CO-adsorbed and TiO_2-supported Pd-Ir nanoalloys are studied at the DFT level

Case study

Client Profile
Tian'e Fan, Visiting student in School of chemistry, University of Birmingham

Contact Details
T.Fan@bham.ac.uk

Product Used
vasp5

Contributors
Prof. Roy L. Johnston

IT Services