World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:18, No:05, 2024

Surface Segregation-Inspired Design for Bimetallic Nanoparticle Catalysts

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Abstract : Bimetallic nanoparticles serve as a promising class of catalysts with tunable properties suitable for diverse catalytic reactions, yet a comprehensive understanding of their actual structures under operating conditions and the optimal design principles remains largely elusive. In this study, we unveil a prevalent surface segregation phenomenon in nearly 100 platinum-group-element-based bimetallic nanoparticles through first principles-based molecular dynamics simulations. Our findings highlight that two components in a nanoparticle with relatively lower surface energy tend to segregate to the surface. Motivated by this discovery, we propose a deliberate exploitation of surface segregation in designing bimetallic nanoparticle catalysts, aiming for heightened stability and reduced consumption of precious metals. To validate this strategy, we further investigate 36 platinum-based bimetallic nanoparticles for propane dehydrogenation catalysis. Through a systematic examination of catalytic sites on nanoparticles, we identify several systems as top candidates with Pt-enriched surfaces, remarkable thermal stability, and superior catalytic activity for propane dehydrogenation. The insights gained garnered from this study are anticipated to provide a valuable framework for the optimal design of other bimetallic nanoparticles.

Keywords : bimetallic nanoparticles, platinum-group element, catalysis, surface segregation, first-principles calculations
Conference Title : ICCMS 2024 : International Conference on Computational Materials Science
Conference Location : Honolulu, United States
Conference Dates : May 02-03, 2024