Optimizing bimetallic alloy catalysts for the cost-efficient reduction of bromate

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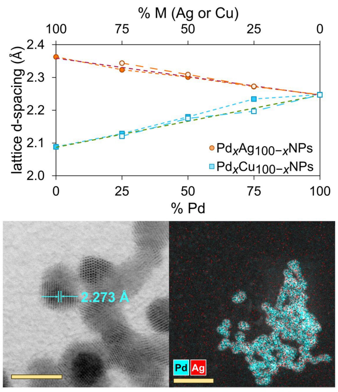
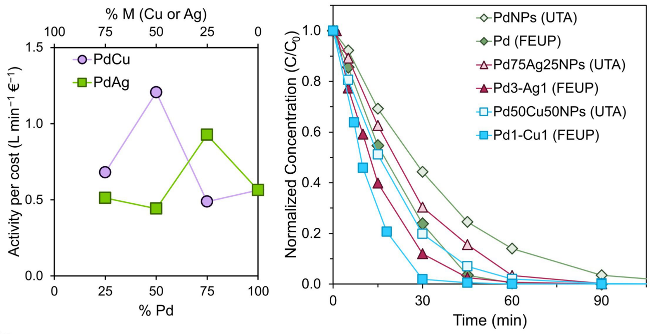
Nanotechnologies

Alloy Nanoparticle Characterization

Pure palladium nanoparticles (PdNPs), palladium–copper nanoparticles (PdCuNPS) and palladium–silver nanoparticles (PdAgNPs) were synthesized by a microwave-assisted polyol method and characterized by a number of techniques. We confirmed that the particles were alloys of the different metals by measuring the lattice d-spacing of the nanoparticles through powder X-ray diffraction (filled circles and squares in top plot) and scanning transmission electron microscopy (open circles and squares in top plot; lower left), as well as energy dispersive spectroscopy (lower right).



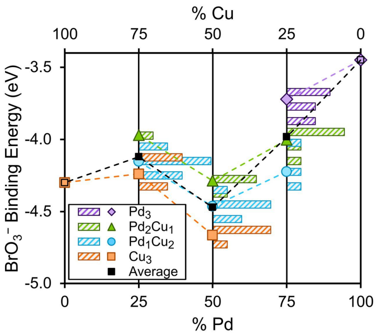
Bromate removal activity



Alloy nanoparticle catalysts with compositions of $Pd_{50}Cu_{50}$ and $Pd_{75}Ag_{25}$ demonstrate significant activity-per-cost improvement versus pure PdNP catalysts (left). Catalysts synthesized using traditional techniques display a similar trend for BrO_3^- reduction activity (right).

Bromate binding energy

Density functional theory (DFT) calculations reveal that alloys create unique surface sites, called ensembles, that change the strength with which BrO_3^- binds to the metal surface.The catalyst activity is related to this binding energy. For PdCuNPs (see right), a 50:50 alloy of Pd – Cu most strongly binds BrO_3^-, which results in the optimal BrO_3^- reduction activity displayed by the $Pd_{50}Cu_{50}$NPs.



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