

Near-surface alloys and Core-shell nanocatalysts for reactions involving hydrogen

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Using first-principles methods, we have identified bimetallic and ternary alloys with specific nano-architecture and significantly improved catalytic properties for a variety of applications, including electrocatalysis for low temperature fuel cells. These near-surface alloys have been synthesized with atomic-layer thickness control in core-shell nanoparticles and, upon experimental testing, have demonstrated remarkable catalytic properties at low temperatures.