Understanding hydrogen uptake by a single palladium nanoparticle

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Andrea Baldi at the DIFFER opening symposium in 2012. Credit: Bram Lamers

A team of four researchers at Stanford University and the Dutch energy research institute DIFFER have determined for the first time the mechanism by which nanometer-sized particles of palladium take up hydrogen. Because the properties of nanoparticles change greatly with their size, choosing the right types of nanoparticle allows you to fine-tune the properties of materials. The finding was published in *Nature Materials* and can lead to improved hydrogen storage and lithium ion batteries.

Getting around the average

Knowing which nanoparticle to pick for an application turns out to be a challenge. "In conventional experiments, researchers produce and measure a whole range of nanoparticles with varying sizes", explains the paper's lead author Andrea Baldi (Stanford University and DIFFER). "However, the difference in behavior between an 8 and 12nm-sized particle is huge. So when you average over a whole group of them, the result does not tell you which behavior belongs to which particle."

The research team, led led by Stanford University's Jennifer Dionne, decided to clear up the relation between nanoparticle sizes and their properties. With the help of Ai Leen Koh at the university's Environmental Transmission Electron Microscope facility, Dionne, Baldi and their fellow researcher Turan C. Narayan managed to select individual nanoparticles and measure how much hydrogen they contain when exposed to varying pressures of hydrogen gas.

Shell model

The team's results fit a model in which an outer shell of the palladium particle loads up on hydrogen first. Absorption of hydrogen causes palladium to swell up by roughly 10%, so the shell expands and pulls open the particle's core to more easily suck in hydrogen. The smaller the particle, the larger the relative influence of the outer shell on its bulk. "Apart from our measurements on hydrogen uptake, this also fits data on nanostructured electrodes for lithium ion batteries. in which smaller particles tend to charge at lower potentials."

Andrea Baldi: "The breakthrough is that we can now measure and potentially predict how an individual particle's size, shape and crystal structure determine its mechanism of hydrogen uptake and release."

Zooming in further

"In our follow-up research, we want to take the next step and look at the way hydrogen is distributed within an individual nanoparticle", says

Baldi. "That should really open up a window on the uptake process."

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