

Palladium, meet copper: Researchers use machine learning to improve catalysts

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Researchers from Skoltech and their colleagues from Germany and the US have studied the properties and behavior of a palladium-copper alloy under changing temperatures and hydrogen concentrations, with highly

relevant implications of this research for catalyst design. The paper was published in the *Journal of Applied Physics*.

Transition metal-alloy materials can have catalytic properties and are widely used in facilitating various chemical reactions such as CO₂ hydrogenation, a process that turns carbon dioxide into methanol. Using an alloy of a more expensive reactive element with another one that is cheaper and more inert makes these catalysts highly efficient. One example of such a catalyst would be an alloy of palladium (Pd) and copper (Cu), where isolated [atoms](#) of Pd are positioned in the Cu lattice.

Zhong-Kang Han, Debalaya Sarker and Sergey Levchenko of the Skoltech Center for Energy Science and Technology (CEST) and their colleagues modeled the properties of a Pd/Cu alloy, using a [machine-learning model](#) to predict the distribution of Pd atoms on a Cu surface as a function of [hydrogen](#) partial pressure and [temperature](#). "Only Pd atoms at the surface provide catalytically active sites. Therefore, it is important to know how many of these atoms can be found at the surface at relevant temperatures and hydrogen partial pressures," Levchenko says.

He says that evaluating the energies of many atomic configurations of Pd within the Cu lattice requires a lot of computational resources, so the researchers chose a surrogate cluster expansion model that is easier to handle. "This model allows us to evaluate the energy of millions of configurations in seconds. In this study, we had a system that is more complex than the ones typically studied using cluster expansion: a surface of an alloy where the stability of various atomic configurations is influenced by adsorbates from the gas phase. Therefore, we applied the machine-learning approach based on compressed sensing (a method widely used to compress images) to develop a very accurate and predictive surrogate model," Levchenko notes.

The team found that hydrogen adsorption indeed has a strong effect on

the concentration of Pd atoms in the top layer of Cu (111) surface.

"While at low hydrogen partial pressures and higher temperatures Pd prefers to stay at the surface, at higher pressures and lower temperatures hydrogen adsorption drives Pd away from the [surface](#)," Levchenko explains.

The authors hope that their findings can open the door for designing metal [alloys](#) with better [catalytic properties](#) by taking into account dynamic changes in the composition and structure of materials at realistic operational conditions.

More information: Zhong-Kang Han et al, First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures, *Journal of Applied Physics* (2020). [DOI: 10.1063/5.0020625](#)

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