High-entropy nanoparticles hold promise for catalytic applications

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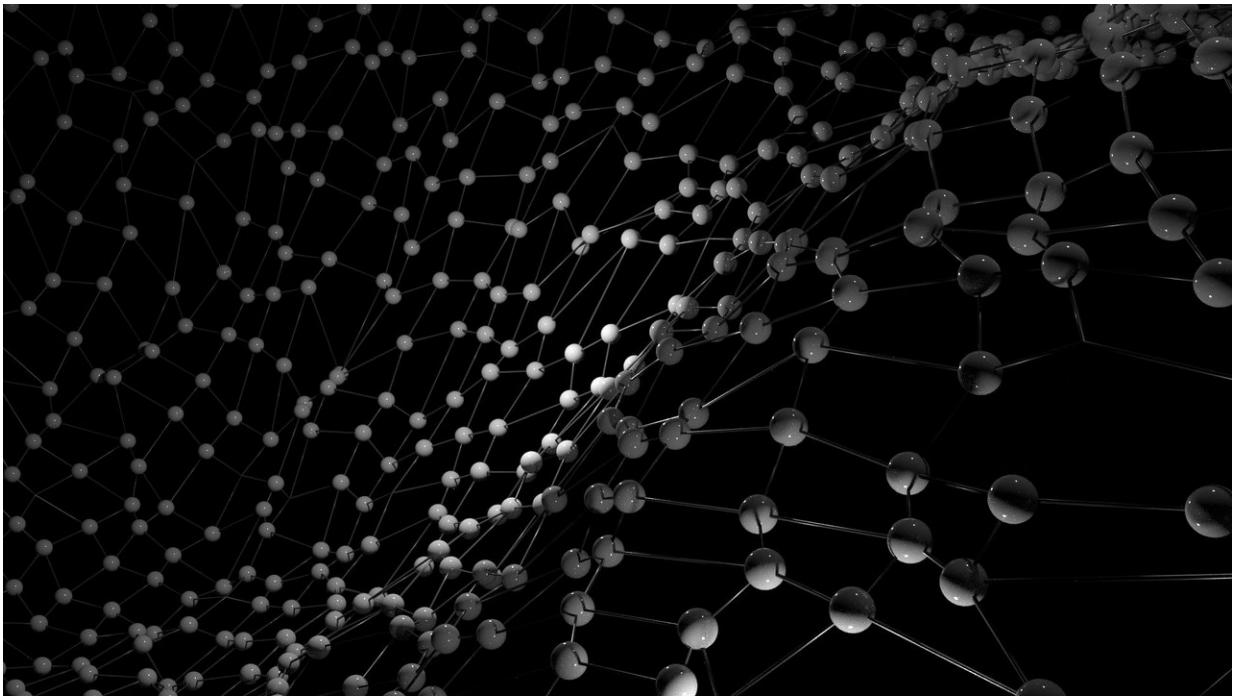

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Alloying is a magic trick used to produce new materials by synergistically mixing at least two metallic elements to form a solid solution. Recent developments in science have found great applications of alloy materials in catalysis, for which nanometer scale bi- or tri-metallic particles are used to accelerate the rate of chemical reactions. But the application of alloys as catalysts is limited by so-called

"miscibility," as not any arbitrary combination of elements can form a homogeneous alloy, neither for robust tuning of the ratio between the two components.

Reported in *Nature Communications* this week, a research team led by Johns Hopkins University researcher Chao Wang, working with collaborators from the University of Maryland, University of Illinois at Chicago, and University of Pittsburgh, uncovered a new method to break through this limitation. In this work, they mix Co and Mo, two elements that are rarely miscible, but which combination is believed to be important for catalyzing energy-relevant chemical reactions, such as decomposition of ammonia. Instead of directly blending them together, Chao and his team added another three ingredients, Fe, Ni and Cu, all of which are earth-abundant transition metals. When the five elements come together in a particle of nanometer large, a single homogeneous solid solution forms that allows for the incorporation of Co and Mo atoms at various ratios. Scientists call this group of materials "high-entropy alloys."

"The trick behind is to increase the disordering, randomness of the way that the metal atoms line up in the alloy crystals," explains Wang, an assistant professor in the Department of Chemical and Biomolecular Engineering at Johns Hopkins Whiting School of Engineering.

The quantity describing this phenomenon is called "entropy" in physics. The quinary alloy nanoparticles created by Wang and his team turn out to possess higher entropy than conventional, relatively simple bi- or tri-metallic alloys. In this unique condition, the atomic characteristics of different elements are rendered and become easier to mix.

The high-entropy alloy nanoparticles are believed to have great potential for catalytic applications.

"Now that we can make alloy nanoparticles of elements that were believed to be immiscible before, we are able to create new, unprecedented catalysts with optimal surface adsorption properties for targeted reactions," said by Pengfei Xie, a postdoctoral fellow in Wang's lab, and first author of the *Nature Communications* paper.

The scientists demonstrated the quinary Co-Mo-Fe-Ni-Cu alloy nanoparticles as superb catalysts for breaking the chemical bond between nitrogen and hydrogen atoms in ammonia, an important way to release hydrogen from this liquid chemical for feeding fuel cells and power future electrical vehicles.

More information: Highly efficient decomposition of ammonia using high-entropy alloy catalysts. *Nature Communications*. doi.org/10.1038/s41467-019-11848-9

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