

# Recipe for nanoparticle interfaces revealed

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At the nanoscale, interfaces between different materials or phases in a structure can have a profound affect on its properties. Now a team of scientists from Northwestern University has come up with a set of basic design rules for the creation of interfaces in nanoparticles made from multiple components [Chen et al., *Science* **363** (2019) 959, <https://doi.org/10.1126/science.aav4302>].

“Interfaces in nanomaterials significantly impact the chemical and physical properties of such structures. However, there is limited understanding of how thermodynamically stable phases form in a nanoparticle and how specific interfaces between them can be constructed,” points out Chad A. Mirkin, who led the work.

His team has developed a technique, which they reported previously [*Science* **352** (2016) 1565], known as scanning probe block copolymer lithography (SPBCL), for the synthesis of polyelemental nanoparticles. The approach uses scanning probe lithography to put attoliter volumes of metal-coordinated block copolymers into specific locations. When the polymers are heated, they act as mini reactors within which single nanoparticles are synthesized.

“Our method allows for the synthesis of polyelemental nanoparticles with unparalleled control over particle composition, size, and position,” says Mirkin.

In their latest work, the team used this approach to create nanoparticles from a mixture of seven elements, Au, Sn, Ag, Pd, Cu,

Ni, and Co (Fig. 1), in combination with density functional theory calculations to predict which interfaces will form.

“By exploring a library of particles containing up to seven elements, we developed a framework of design rules to guide the synthesis of polyelemental nanoparticles with specific interfaces,” explains Mirkin.

The team found that complex phase-separation phenomena are at work determining whether particles of two, three, or four phases are formed. The interfaces that arise in a polyelemental nanoparticle will depend upon the interfacial energy between phases and surface energies. The nanoparticles that the team produced show a variety of interfaces and combinations of interfaces.

“A nanoparticle comprising specific phases finds its most stable construction when the total interfacial and surface energy are minimized, which serves as the governing rule for the design of polyelemental nanoparticle interfaces,” states Mirkin. “Understanding how specific classes of interfaces can be established in a single particle will be an important step for designing novel and functional particles.”

For example, for a nanoparticles with ‘*n*’ phases, there will be between  $(n-1)$  and  $n(n-1)/2$  interfaces, the team calculated. They also observed that biphasic structures do not predict the architecture of particles with three or more phases. Furthermore, if an

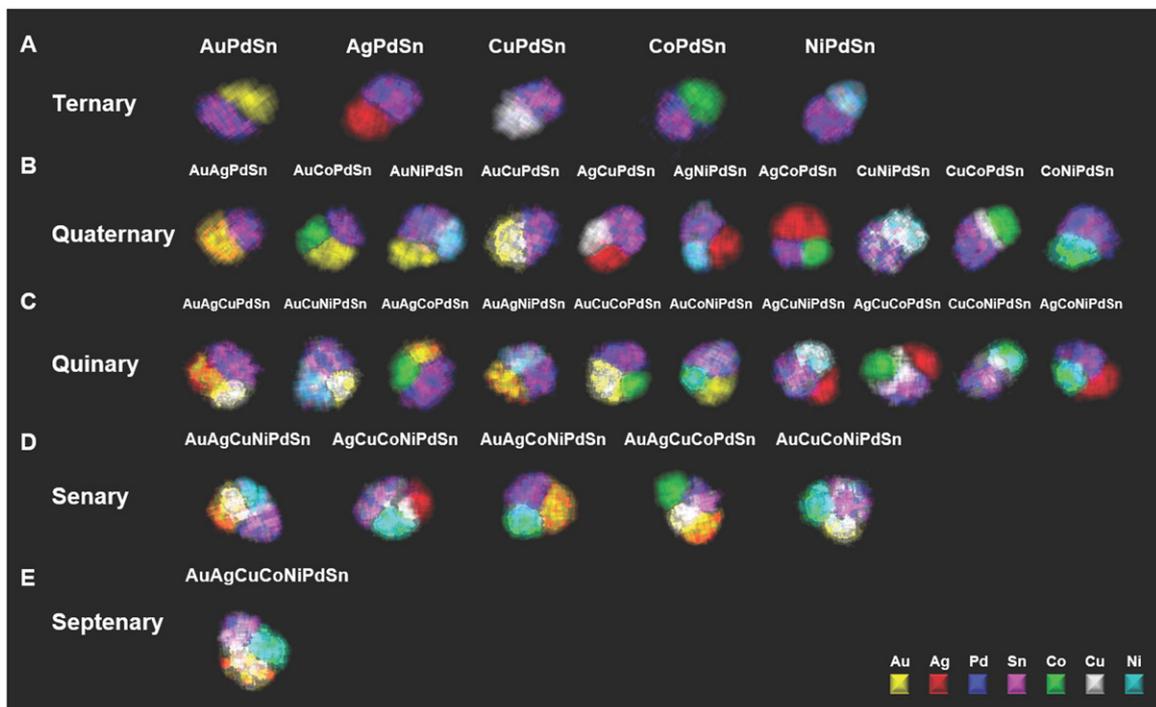


Fig. 1. A seven-element library of multi-phase heterostructured nanoparticles that utilize PdSn as the basic building block.

interface is not seen in a tri-phase nanoparticle, it will not occur in higher order nanoparticles.

“Our work will be a fundamental driver for designing novel polyelemental nanoparticles for many applications,” Mirkin told *Nano Today*. “Eventually, polyelemental nanoparticles with optimized interface structures may have applications spanning catalysis, plasmonics, nanoelectronics, and energy harvesting.”

The team’s approach could help find just the right nanoparticle for a particular application as so many different combinations of particle size, composition, and position can be generated.

“If SPBCL is combined with a massively parallel patterning technique such as polymer pen lithography (PPL), millions of probes over centimeter-scale areas could be used to generate millions of different polymer nanoreactors simultaneously,” he explains. “This provides a powerful platform for nanocombinatorics, where new nanoparticle compositions, including those that are not easily accessible by conventional techniques, can be generated, characterized, and screened.”

Luis M. Liz-Marzán, scientific director of CIC biomaGUNE in Spain, believes that the work shows just what rational engineering of the distribution of different metals in a nanoparticle can achieve.

“By taking a combinatorial approach to particle design, together with annealing, the elemental distribution and strain can be engineered, which may have large relevance in various fields and in catalysis in particular,” he says Alexander Govorov of the University of Ohio agrees that the work makes an important contribution to the field of multi-component nanocrystals. “The importance of the dimension of a nanoparticle is well known since the surface-to-volume ratio is one of the key parameters of catalysis,” he points out. “But this work brings another parameter, which could potentially lead to more efficient catalysis and photocatalysis: multi-component structure with interfaces transparent for charge transfer.”

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## Transition metal nanobelts show high conductivity

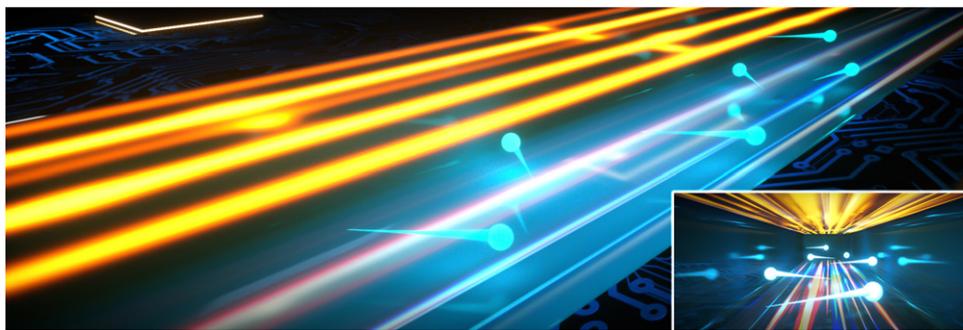
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Two-dimensional materials usually boast high carrier mobility when the carrier density is low. But now researchers have fabricated nanobelts of the transition metal NbAs that show high mobility even when the carrier density is also high [Zhang et al., *Nature Materials* (2019), <https://doi.org/10.1038/s41563-019-0320-9>].

If conventional bulk metals are reduced to the nanoscale, conductivity decreases because surface roughness and defects scatter the charge carriers, reducing their overall mobility. Recently, however, a new type of topological materials called Weyl semimetals have been discovered. In single crystals of these exotic materials, the conduction and valence bands touch at specific points leading to unusual electronic properties and phenomena.

Now a team from Fudan University, the High Magnetic Field Laboratory of the Chinese Academy of Sciences in Heifei, Nanjing University of Science and Technology, Beijing University of Technology, the University of Queensland, Brisbane, ETH Zurich, Trinity College Dublin, and University of California, Davis has designed a new way of synthesizing the Weyl semimetal NbAs. Their approach is based on chemical vapor deposition, taking advantage of the reaction between the metal chloride  $\text{NbCl}_5$  with hydrogen at high temperatures and low pressures. When carried out in an As atmosphere with a thin (15 nm) Au layer acting as a catalyst, nanobelts of NbAs are produced.

The NbAs nanobelts are highly crystalline, with a large proportion of (001) surfaces, and can be regarded as a three-dimensional



**Fig. 1.** Sketch of ultrahigh conductivity in NbAs nanobelts. The surface state of NbAs nanobelts is found to host the largest sheet conductivity. The electrons are mostly transported through surface states without encountering large-angle scattering.