Research predicts size-induced transition to nanoscale half-metallicity

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How big does a cluster of metal atoms actually have to be before it starts acting like a metal: ductile, malleable and a conductor?

The emergence of metallic attributes, usually referred to as the transition to metallicity, is among the most intricate aspects of the size evolution of properties of atomic clusters that are metals in bulk quantities. Researchers at Argonne and other research centers worldwide are looking for answer to this question, which is central for establishing limits of miniaturization in nanoelectronic devices.

An even more intricate question is whether researchers can identify a nanoscale analog of the bulk half-metallic state and the size-driven transition to that state.

A recent study by Argonne theorists suggests that the answer to this question is yes. Their work represents the first prediction of a nanoscale analog of the bulk half-metallic state.

In distinction from normal metals, in which electrons with alpha and beta spins carry the electrical current, half metals are elements or compounds with spin-polarized conductivity. Electrical current in half metals translates into spin transport, which lies at the foundation of spintronics technology. Scientists in the field of spintronics study how to use “spin” or magnetic properties of particles, such as electrons, to develop novel and better sensors, recording devices, switches and quantum computers.

Even the common metallic state becomes a complex phenomenon at the nanoscale, Julius Jellinek of Argonne's Chemical Science and Engineering Division.

“Small or medium atomic clusters of metallic elements may lack all attributes normally associated with the bulk metallic state,” he said. “These attributes then grow in as clusters grow in size. The same should be true of the half-metallic state, and our research shows that it is.”

The Argonne theorist collaborated with an experimental group at the Johns Hopkins University led by Kit Bowen, Jr. The experiments have indicated that, as a small, negatively charged manganese cluster grows, the gap between the energies of its two most external electrons decreases and closes when the cluster size reaches six atoms.

Computations and subsequent analysis by Jellinek and his colleagues revealed that the closure of the gap between the electron energy levels takes place in one spin manifold, but not the other. This spin-polarized nature of the energy gap closure is what constitutes the nanoscale analog of the bulk half-metallic state. Understanding the finite-size analog of the bulk half-metallicity and the size-driven transition to it is central for many areas of nanoscience and nanotechnology, in particular nanospintronics.

The prediction of finite-size half-metallicity must still be tested experimentally using future spin-polarized photoelectron spectroscopy measurements. “The finite-size analog of half-metallicity may be more ubiquitous than the bulk half-metallic state,” Jellinek said. “Nanoscale half-metallicity may emerge as a transient state in the size-driven evolution of properties of systems even for elements and substances that are not half-metals in bulk quantities.”

The study was published in the journal Physical Review B and republished by the *Virtual Journal of Nanoscale Science and Technology*. Collaborators on this research were Julius Jellinek, Paulo H. Acioli and Juan Garcia-Rodeja from Argonne National Laboratory, and Weijun Zheng, Owen C. Thomas and Kit Bowen, Jr. from the Johns Hopkins University.

Source: Argonne National Laboratory

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