Uncertainty gives scientists new confidence in search for novel materials

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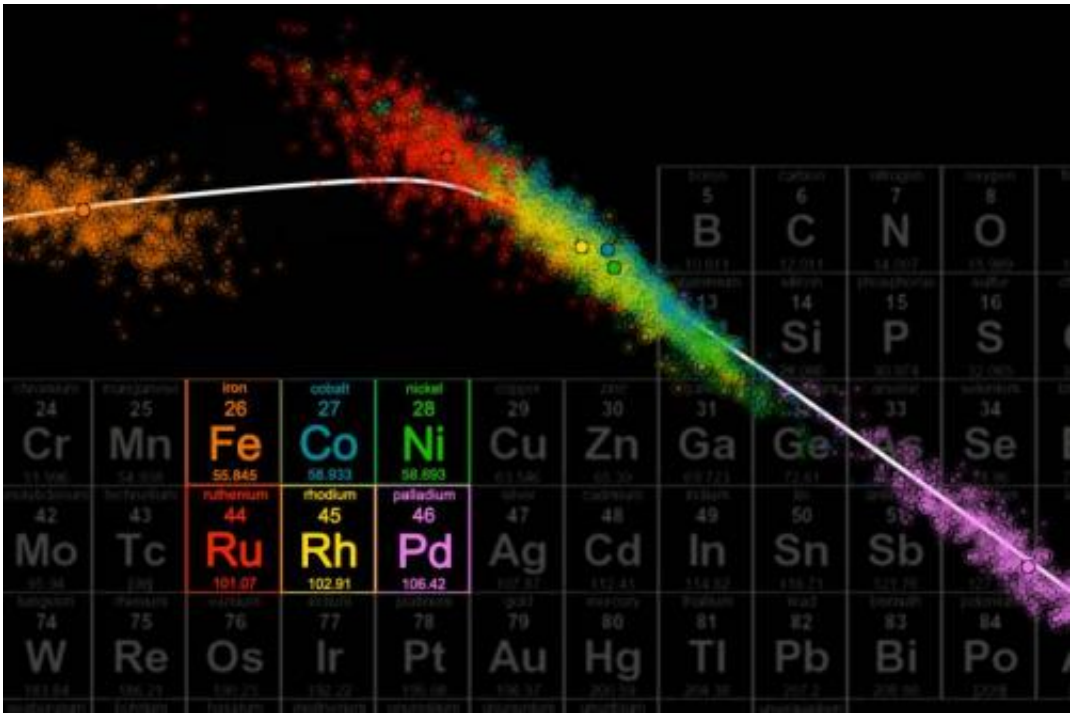

This image shows the results of calculations aimed at determining which of six chemical elements would make the best catalyst for promoting an ammonia synthesis reaction. Researchers at SLAC and Stanford used Density Functional Theory (DFT) to calculate the strength of the bond between nitrogen atoms and the surfaces of the catalysts. The bond strength, plotted on the horizontal axis, is a key factor in determining the reaction speed, plotted on the vertical axis. Based on thousands of these calculations, which yielded a range of results (colored dots) that reveal the uncertainty involved, researchers estimated an 80 percent chance that ruthenium (Ru, in red) will be a better catalyst than iron (Fe, in orange.) Credit: Andrew Medford and Aleksandra Vojvodic/SUNCAT, Callie Cullum

Scientists at Stanford University and the Department of Energy's SLAC National Accelerator Laboratory have found a way to estimate uncertainties in computer calculations that are widely used to speed the search for new materials for industry, electronics, energy, drug design and a host of other applications. The technique, reported in the July 11 issue of *Science*, should quickly be adopted in studies that produce some 30,000 scientific papers per year.

"Over the past 10 years our ability to calculate the properties of materials and chemicals, such as reactivity and mechanical strength, has increased enormously. It's totally exploded," said Jens Nørskov, a professor at SLAC and Stanford and director of the SUNCAT Center for Interface Science and Catalysis, who led the research.

"As more and more researchers use computer simulations to predict which materials have the interesting properties we're looking for – part of a process called 'materials by design'—knowing the probability for error in these calculations is essential," he said. "It tells us exactly how much confidence we can put in our results."

Nørskov and his colleagues have been at the forefront of developing this approach, using it to find better and cheaper catalysts to speed ammonia synthesis and generate hydrogen gas for fuel, among other things. But the technique they describe in the paper can be broadly applied to all kinds of scientific studies.

Speeding the Material Design Cycle

The set of calculations involved in this study is known as DFT, for Density Functional Theory. It predicts bond energies between atoms based on the principles of quantum mechanics. DFT calculations allow

scientists to predict hundreds of chemical and materials properties, from the electronic structures of compounds to density, hardness, optical properties and reactivity.

Because researchers use approximations to simplify the calculations – otherwise they'd take too much computer time – each of these calculated material properties could be off by a fairly wide margin.

To estimate the size of those errors, the team applied a statistical method: They calculated each property thousands of times, each time tweaking one of the variables to produce slightly different results. That variation in results represents the possible range of error.

"Even with the estimated uncertainties included, when we compared the calculated properties of different materials we were able to see clear trends," said Andrew J. Medford, a graduate student with SUNCAT and first author of the study. "We could predict, for instance, that ruthenium would be a better catalyst for synthesizing ammonia than cobalt or nickel, and say what the likelihood is of our prediction being right."

An Essential New Tool for Thousands of Studies

DFT calculations are used in the materials genome initiative to search through millions of solids and compounds, and also widely used in drug design, said Kieron Burke, a professor of chemistry and physics at the University of California-Irvine who was not involved in the study.

"There were roughly 30,000 papers published last year using DFT," he said. "I believe the technique they've developed will become absolutely necessary for these kinds of calculations in all fields in a very short period of time."

Thomas Bligaard, a senior staff scientist in charge of theoretical method

development at SUNCAT, said the team has a lot of work ahead in implementing these ideas, especially in calculations attempting to make predictions of new phenomena or new functional materials.

More information: "Assessing the reliability of calculated catalytic ammonia synthesis rates" A.J. Medford, et al., *Science*, 11 July 2014. DOI: 10.1126/science.1253486

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