The University of Texas at San Antonio

UTSA. Physics and Astronomy

Using Machine Learning to Prospect for New Magnetic Materials

Friday, February 9, 2024 at 11:00 AM

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Magnetic materials are essential for energy generation and information devices. They also play an important role in advanced technologies and green energy economies. Most commercial magnets contain rare earth elements, considered a critical resource. An outstanding challenge of notable scientific interest is the discovery and synthesis of novel magnetic materials that do not contain rare earth elements yet meet the performance and cost goals for advanced electro-magnetic devices. I will discuss the synthesis of a heretofore unknown rare earth-free magnetic compound by integrating machine learning, an adaptive genetic algorithm, first-principles calculations, and experimental synthesis. Magnetic measurements show that this newly discovered material exhibits a high magnetic anisotropy and saturation magnetic polarization, which is suitable for permanent-magnet applications. Our machine learning-guided approach presents a promising pathway for efficient materials design and discovery and can be applied to the search for other functional materials.

Bio: Jim Chelikowsky received a BS from Kansas State University and a PhD from the University of California at Berkeley, both in physics. Before assuming the "Tex" Moncrief Chair in Computational Materials at Texas in 2005, he worked at the University of Minnesota for almost 20 years. His research is focused on computational applications of quantum theory to understand, design, and discover properties of materials. His work has been recognized by the David Turnbull Award from the Materials Research Society, the David Adler Award and the Aneesur Rahman Prize from the American Physical Society, the John Bardeen Award from the Minerals, Metals & Materials Society, and most recently, the Feynman Prize in Theory from the Foresight Institute. He is a fellow of the Materials Research Society, the American Physical Society, and the American Association for the Advancement of Science.

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