QMC simulations reveal magnetic properties of titanium oxide material

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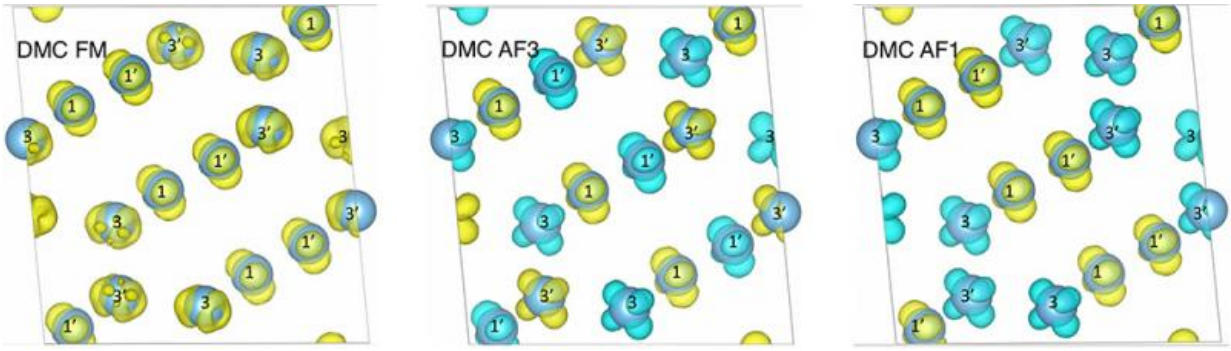

Diffusion Monte Carlo spin densities for low-temperature Ti4O7 ferromagnetic (left), antiferromagnetic 3 (center), and antiferromagnetic 1 phases. Yellow represents a positive spin density (or spin up) and blue represents a negative spin density (or spin down). Credit: Anouar Benali and Olle Heinonen, Argonne National Laboratory

By running computationally intensive quantum Monte Carlo simulations at the Argonne Leadership Computing Facility (ALCF), a U.S. Department of Energy (DOE) Office of Science User Facility, researchers have demonstrated the ability to accurately calculate the magnetic properties of a titanium oxide material that exhibits useful properties for renewable energy and computing technologies.

Your house is likely littered with titanium dioxide (TiO_2), from the paint on your walls, to the sunscreen and toothpaste in your bathroom, to the

papers on your desk. A brilliant white powder, titanium dioxide is a transition metal oxide that has many favorable properties including optical and catalytic ones.

"Titanium oxides are versatile transition metal compounds that may be used for a range of applications, including electronic devices and photocatalysis," said Olle Heinonen, materials scientist at Argonne National Laboratory.

While titanium dioxide may be the most well-known titanium oxide material, one of its derivatives, Ti_4O_7, is another material of interest due to its potential applications in resistive memories and oxide-based fuel cell electrodes. To explore such applications, scientists need to better understand its electronic and magnetic properties.

With the computational power of Mira, the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer, researchers have, for the first time, accurately calculated the magnetic properties of Ti_4O_7 with quantum Monte Carlo (QMC) simulations.

The team's results, published in *Physical Chemistry Chemical Physics*, reveal the Ti_4O_7 ground state—the material's properties at the lowest possible energy state. By accurately computing the ground state, researchers are able to determine or infer many important material properties, such as crystal structure, conductivity, and magnetism.

"Calculating the ground state is crucial for computational predictions of a material's behavior in realistic conditions in which temperature, pressure, and time can change its structure," said Anouar Benali, ALCF computational scientist and lead author of the study.

Because Ti_4O_7 has several magnetic states close in energy, scientists were previously unable to conclusively determine the ground state

through experiment or other computational methods, such as density functional theory (DFT). However, with access to Mira, the research team was able to perform QMC calculations that helped settle the long-standing uncertainty with Ti_4O_7 by identifying the three magnetic phases that compromise the material's ground state.

Although QMC requires as much as 1,000 times the computing power of a typical DFT calculation, the method is able to accurately calculate the complex interactions between many electrons. Due to its computational expense, QMC simulations were once limited to modeling systems of small atoms or molecules, but the emergence of supercomputers like Mira has now made it possible to use QMC for rigorous calculations on more complicated materials.

For the Ti_4O_7 study, researchers used the QMCPACK application developed by Argonne, Oak Ridge, Sandia, and Lawrence Livermore national laboratories. By rewriting the most computational intensive parts of QMCPACK using compiler specific extensions (called vector intrinsics) to better utilize the IBM Blue Gene/Q processor, ALCF computational scientists, including Benali, Ye Luo, and Vitali Morozov, were able to improve QMCPACK performance on Mira by 30 percent. Additionally, by rewriting code to use single precision instead of double precision in key data structures, they decreased the amount of data that needed to be stored in memory by 45 percent.

"These code improvements allowed us to study larger electronic systems in a shorter amount of time," Benali said.

More information: Anouar Benali et al. Quantum Monte Carlo analysis of a charge ordered insulating antiferromagnet: the TiOMagnéli phase, *Phys. Chem. Chem. Phys.* (2016). DOI: 10.1039/C6CP02067D