BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: Illinois/232.8 Knh

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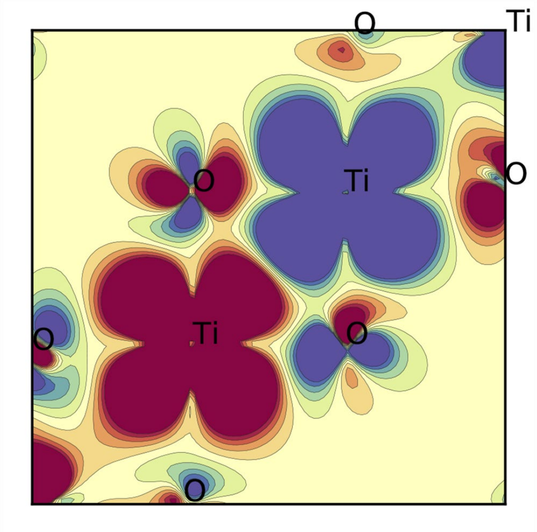
Physics & Engineering

QUANTUM MAGNETS AND MODELS



The spin density in $MgTi_2O_4$. Red indicates a net spin-up in a region, while blue indicates a net spin-down. The excitation predicted flips of both spin regions up. The ground state is a quantum superposition of one region up/the other region down with the exchanged configuration.

Research Challenge

Quantum magnetism describes the behavior of single atoms as they act like tiny bar magnets. There is a great deal of interest and science being conducted to look into different materials and how the atoms of specific materials spin hopefully leading to breakthrough discoveries in materials science that would allow for things like room temperature superconductors. Thanks to high-performance computers such as Blue Waters, it is possible to accurately compute the properties of interacting electronic systems using a quantum Monte Carlo method.

Methods & Codes

This project has developed a new technique that maps interacting quantum simulations to coarse-grained models. This requires quantum Monte Carlo simulations that can compute the necessary matrices. To perform the quantum Monte Carlo calculations, the QWalk package was used, a package developed at the University of Illinois at Urbana-Champaign.

Results & Impact

The goal of this work was to produce a prediction of the singlet excitation in the material $MgTi_2O_4$. (A Spinel Oxide). A solid prediction was made with these simulations that will be tested via direct experiment. In the figure, it shows the computed spins, which, when they flip to the same direction, will produce the excitation.

Why Blue Waters

The Blue Waters project staff helped optimize the code used in the calculation. The Blue Waters Symposium (BWS) was an excellent research forum that illuminated modern coding practices such as using the Travis CI based on conversations at the BWS.