

拡散モンテカルロを使用した LiVX₂ システムの基底状態決定

Ground state determination of LiVX₂ system using Diffusion Monte Carlo

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The LiVX₂ system (X: O, S, Se) is an example of a Heisenberg antiferromagnet with the geometrical frustration existing on the triangular lattice of its vanadium layer. This class of system is often a host to exotic electronic states, such as the valence-bond solid (VBS) state. Occurring especially at lower temperatures, the formation of this state is experimentally detectable by a metal-to-insulator transition coupled with trimerization of the triangular vanadium lattice. While LiVO₂ and LiVS₂ has been experimentally observed to exhibit this transition, LiVSe₂ keeps its metallicity to low temperatures without showing signs of the transition.

With strong electronic correlation characterizing the system, methods based on one-body theory such as density functional theory (DFT) often fail to reliably predict its properties. Our preliminary calculations revealed that conventional DFT predicted trimerization of all three compounds, which is

inconsistent with the experimentally observed preference. Attempts to improve the electronic structure by the addition of Hubbard U terms instead resulted in non-trimerized structures for all three compounds, which is equally incorrect.

In this work, we employed Diffusion Monte Carlo (DMC), a method based on true many-body wave function and thus is expected to capture electronic correlation more reliably. We performed static energetic comparison between trimerized and non-trimerized structures of LiVX₂, as optimized by the DFT calculations. We also seek to clarify the true nature of the insulating ground state by comparing the energetics and performing charge density analysis on the DMC wavefunctions with the nodal structures of spin-polarized and non-spin-polarized DFT trial wavefunctions. We are going to present our current results and discuss their implications

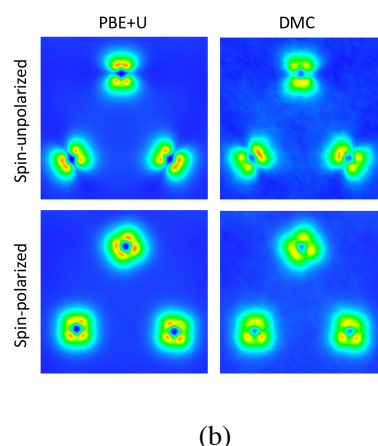
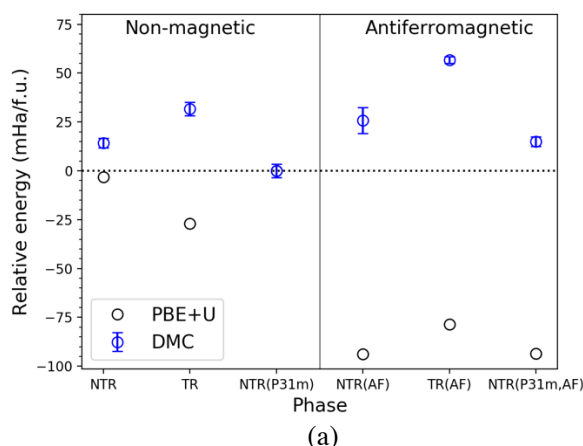


Figure 1. a) Total energies relative to the non-trimerized (NTR) P31m phase of LiVS₂ from DFT(PBE+U) and DMC. The AF phases are strongly preferred in DFT, with reversed preference for trimerization, in contrast to the DMC data. b) Total charge density from all spins of the V trimer as calculated by DFT(left) and DMC(right).