DFT and DMFT study of magnetism of ternary chromium tellurides under pressure

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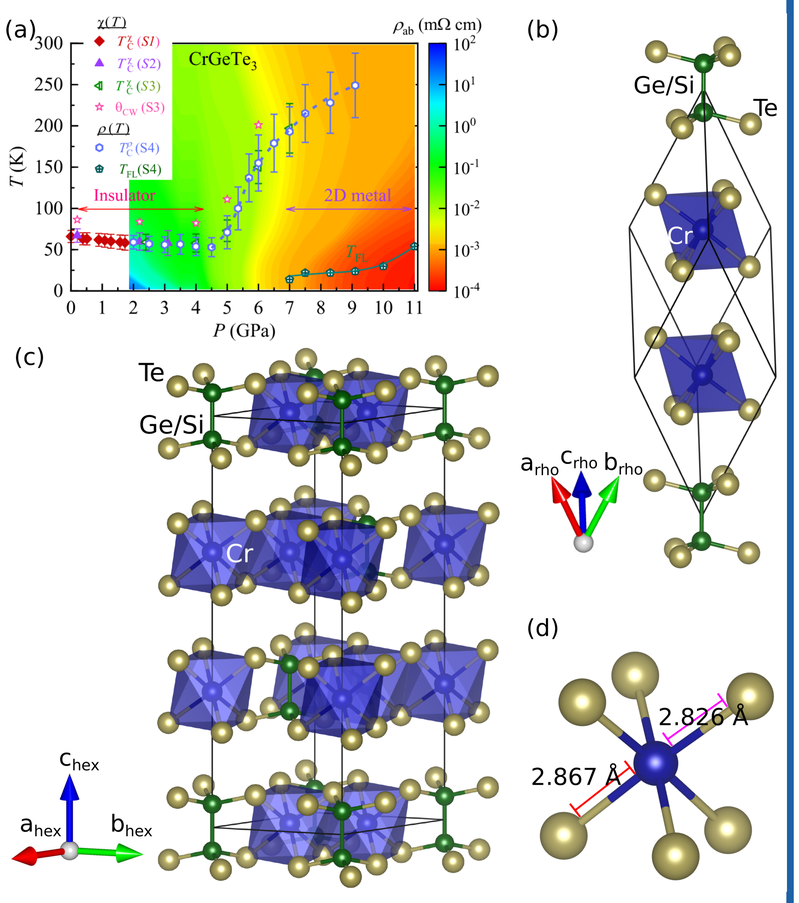
1. Introduction

Background

- Two-dimensional long-range ferromagnetism was discovered in a number of van der Waals crystals, for example $CrGeTe_3$ [1].
- A pressure-induced insulator-metal transition of $CrGeTe_3$ was discovered. A phase diagram is shown in panel (a), cited from Ref. [2].

Motivation

- We are theoretically investigating the insulator-metal transition.
- We computerize Curie-Weiss temperature θ_{CW} and other physical quantities to compare with the experimental phase diagram.



6. Conclusions

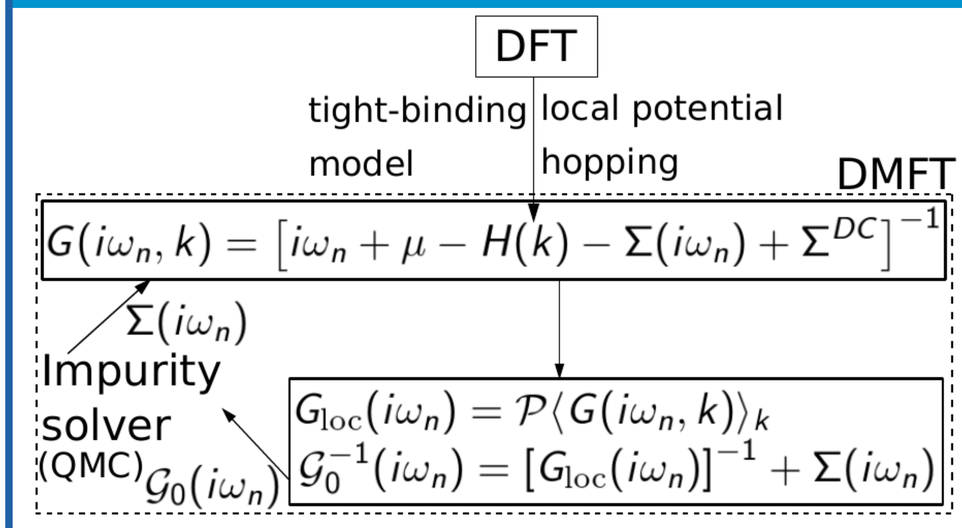
- The insulator-metal transition is studied theoretically.
- By DFT with GGA+U, the pressure dependent Curie-Weiss temperature θ_{CW} is calculated.

7. References

[1] C. Gong and *et al.*, Nature **546**, 265 (2017).

[2] D. Bhoi and *et al.*, Phys. Rev. Lett. **127**, 217203 (2021).

2. Methods



Methods

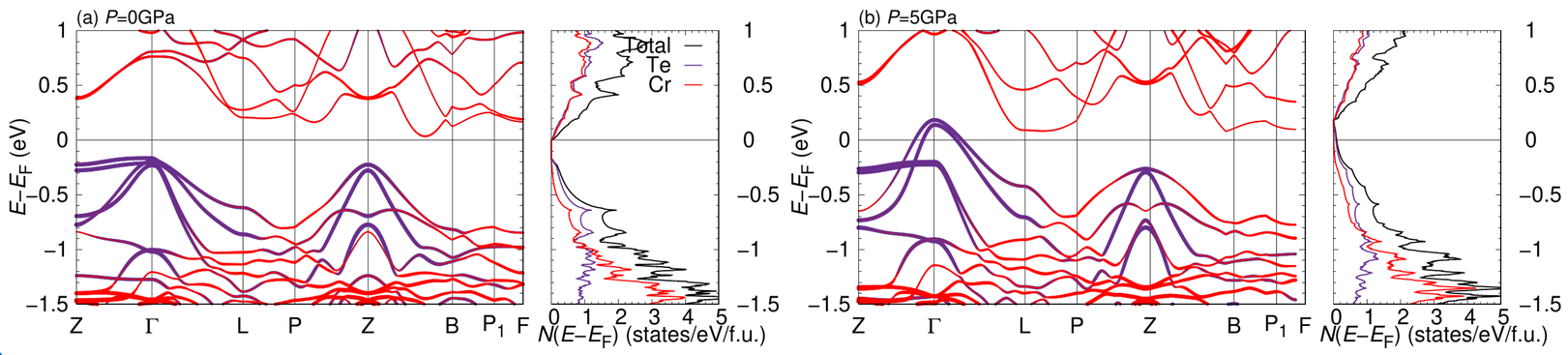
- Density functional theory (DFT)
- DFT with generalized gradient approximation (GGA) + U
- Dynamical mean-field theory (DMFT)

To study

- electronic structure by DFT using full potential local orbital (FPLO) basis
- exchange couplings and Curie-Weiss temperature θ_{CW} by using DFT with GGA+U to apply energy mapping in Heisenberg model
- spectral function by solving the multi-orbital Hubbard model using Integrated DMFT software for Correlated electrons (DCore)

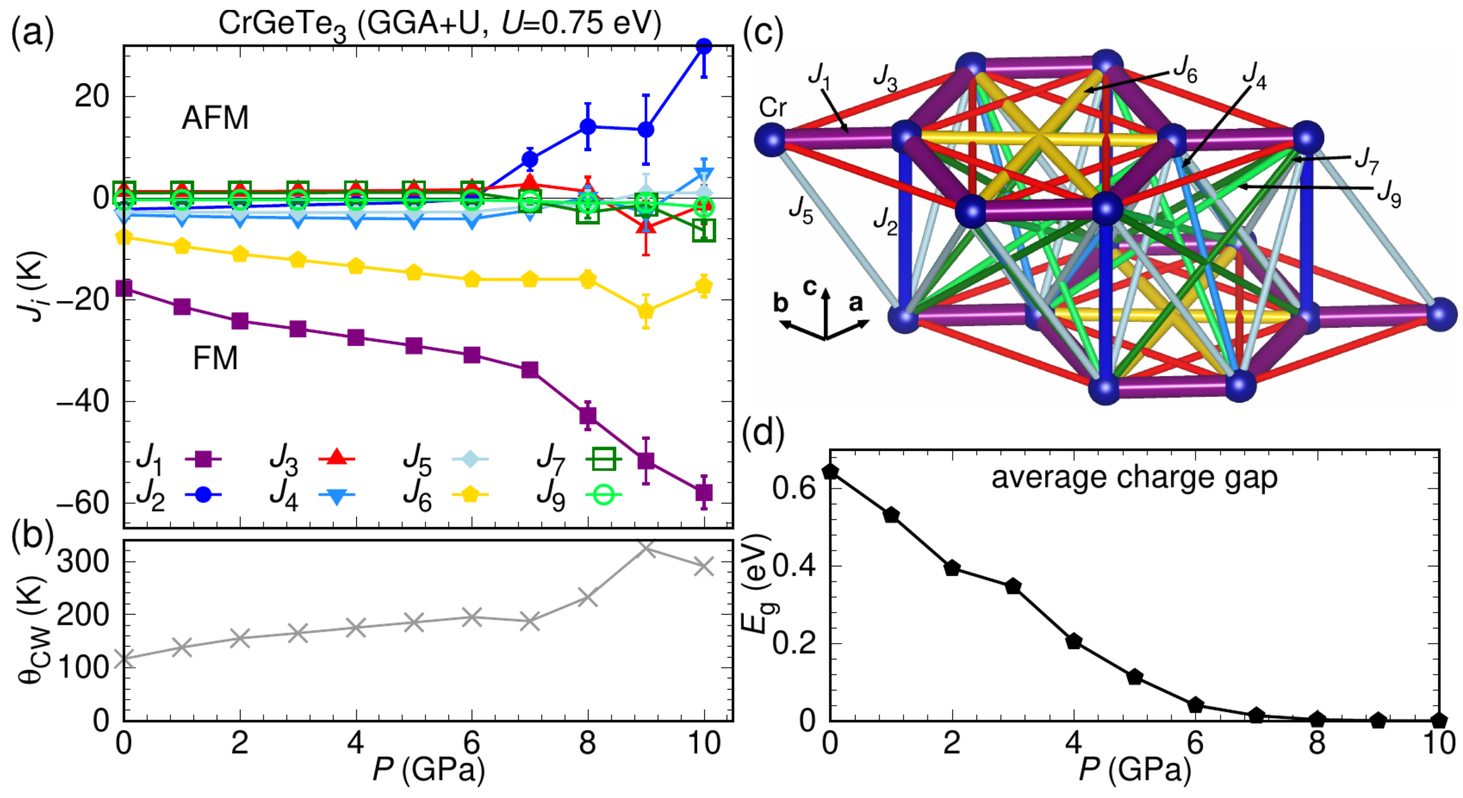
3. Result I: Electronic structure

In DFT calculations, the band structure and density of states directly show the insulator-metal transition between 0GPa in panel (a) and 5GPa in panel (b).



4. Result II: Curie-Weiss temperature

Applying energy mapping within GGA+U, the evolution of exchange couplings is shown in panel (a) and illustration of exchange paths is shown in panel (c).
In panel (b), by using the exchange couplings, the evolution of Curie-Weiss temperature θ_{CW} is calculated, which is comparable to the experimental result in Ref. [2].
In panel (d), the insulator-metal transition is seen in the average charge gap.



5. Result III. Spectral function

By DMFT, we get the spectral function of ferromagnetic $CrGeTe_3$ at 0GPa and finite temperature (100K) to approach the insulating state, which can be compared with angle-resolved photoemission spectroscopy in experiment.