

Project Title:

Quantum phase transition of Chromium (Cr) under high pressure

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1. The spin density wave of Chromium under high pressure is studied by the first principle calculation. The bcc chromium is typical antiferromagnet with itinerant electron, and it presents quantum phase transition under high pressure. This project is funded by Grant-in-Aid for Scientific Research on Innovative Areas 'Earth science based on the high pressure and temperature neutron experiments' (No. 20103001-20103005) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.
2. The derivation of spin density wave and electronic correlation of Chromium under high pressure is studied by VASP, PWSCF and Wien2k.
3. Several phases will present under high pressure at low temperature. The wave vector of spin wave will get short under high pressure, and the wave vector will get long if the pressure is increased further.
4. The results also show the magnetic structures of Cr are very sensitive to the lattice constant and the choice of the Hubbard U parameter. The electronic of the magnetic phases at ambient pressure can be described adequately with the spin-polarized local density approximation with a small effective Hubbard parameter. The effect of increase electron correlation at high pressure mimic by larger U values helps to rationalize the recently observed quantum phase transition.
5. The Hubbard U will calculated by constrained DFT to check our results, the crystal structure transition under high pressure will be studied. The DMFT calculation will be done to check our results.
6. I wish to extend my account, since some achievement is done now and the result is very important. The result will be checked using other codes and the electronic correlation under high pressure will be studied in detail. The band and electronic structure under high pressure will be studied with wannier and HSE function.

