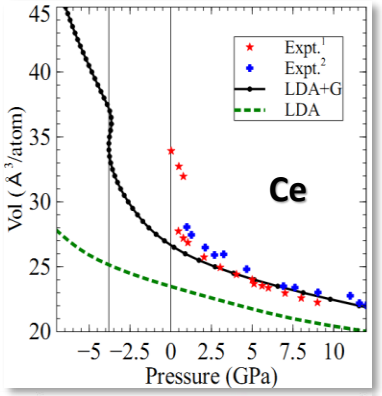
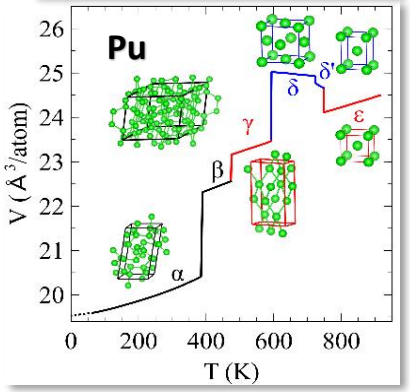
Gutzwiller density functional theory for correlated-electron materials

Scientific Achievements:

Newly-developed LDA+Gutzwiller (LDA+G) method enables accurate and efficient calculation of strongly corelated materials.

- Isostructural volume collapse transition in Ce.
- A series of exotic volume-expansion-collapse transitions in Pu.
- Good description of UO_2, a typical orbital-selective Mott insulator.



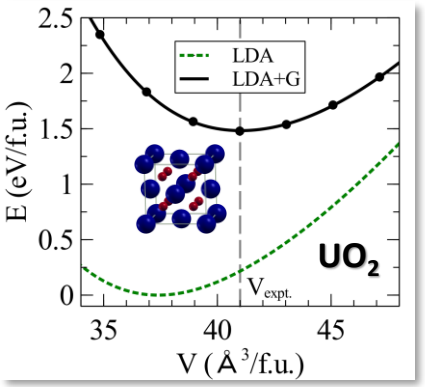


Scientific Impact:

- **Kohn-Sham DFT, workhorse for material simulations, fails for correlated materials.**
- **LDA+G provides an accurate and efficient way to calculate real correlated materials.**

Future direction:

✓ **First-principles Gutzwiller density functional theory without adjustable U and J parameters**



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