Correlated First-principles Study of the Mott Transition in (Sr, Ca, La, Y)VO_3

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Strongly correlated materials exhibit a wide variety of unusual electronic and magnetic properties such as high-temperature superconductivity, metal-insulator transitions, multiferroicity and many more. Studying and predicting such properties could directly lead to important technological improvements. However first-principles schemes relying on a one-electron picture are incompatible with these many-body effects. Fortunately, the combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) offers the possibility to incorporate the effects of local electronic correlations in a first-principles calculation [1, 2]. In this poster, we present a new functionality of the ABINIT package which enables the user to link an external python script to treat electronic correlations. We used the CTHYB solver from the TRIQS package [3, 4] to study the Mott transition in the Mott-Hubbard series (Sr, Ca, La, Y)VO_3.

References

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