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Cluster Impurity Solver for LDA+DMFT Calculations QUAN YIN, SERGEY SAVRASOV, University of California, Davis, CA 95616 TEAM —
We report the electronic structure calculations of strongly correlated systems such as Mott Insulators, using the LDA+DMFT method. LDA+DMFT is a combination of the Density Functional Theory and the Dynamical Mean Field Theory featuring both the one-electron approximation and the many-body treatment for electrons, which is suitable for any ratio of coulomb repulsion over band width, and all computations are self-consistent. In the process of solving the Anderson Impurity Model for DMFT, several solvers with different accuracy were used and their results are compared. This presentation will focus on our most recently developed cluster solver and its applications.

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