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Density Functional Plus Dynamical Mean Field Theory of Correlated Oxides[1]

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The density functional plus dynamical mean field method is outlined and a few recent successes including applications to spin crossover molecules, oxide superlattices and metal-insulator transitions in bulk transition metals are outlined. Insights from the method into the essential role played by lattice distortions (both rotations and bond length changes) in determining the phase diagrams of correlated materials are presented. The key theoretical issue of the double counting correction is outlined, different approaches are compared, and a connection to the energy level differences between strongly and weakly correlated orbitals is presented. Charge transfer across oxide interfaces shown to depend crucially on the double counting correction, suggesting that experiments on oxide superlattices may provide insights into this important problem. Future directions are discussed. This work is performed in collaboration with Jia Chen, Hung Dang, Hyowon Park and Chris Marianetti.

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