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### **First-principles design of magnetic oxides**

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First-principles design of magnetic oxides is one of most ambitious challenges in modern computational physics. The electronic and magnetic properties of these materials are substantially affected by strongly localized electrons, complex crystalline structures, and mixed valencies of magnetic ions. In my talk I shall present an ab-initio Green function method within density functional theory which provides an accurate description of the electronic structure of these materials. In particular, the treatment of strongly localized electrons is improved considerably by applying a self-interaction correction (SIC), thereby removing the spurious interaction of an electron with itself. By localizing a particular electronic configuration using the SIC, we simulate various valencies of magnetic ions. A mixed-valency state can then be efficiently treated within the coherent potential approximation which is implemented in our multiple-scattering Green function code that can be used as well for simulations of any kind of substitutional disorder. In my talk I shall demonstrate the power of our approach on complex magnetic oxidic surfaces and interfaces. In particular, I shall discuss effective exchange interactions in systems with mixed valency and the influence of structural imperfections, such as defects and relaxations, on the electronic and magnetic properties of these materials.