DFT modelling of nano and macro properties of energy viable oxides

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Metal oxides represent a growing asset in many energy related industries due to their chemical, physical, and electronic properties on one hand and their commercial appeal on the other. Metal oxides are massively produced for batteries for mobile and vehicular applications, they receive considerable attention as electro-catalysts for fuel cells and photovoltaic applications, and notably, actinide oxides are used as nuclear fuels for massive energy production. Theoretically, the unifying motif of these different families of materials used in energy storage and generation devices is their complex electronic structure comprising the mixing of the metal and the oxygen electronic bands, which is also responsible for their performance traits related to structure, charge conduction and reactivity.

In this talk I will show how first principles atomistic modelling is used to understand the structure property relationship in energy viable oxides, ranging from modern batteries and fuel cell components to nuclear fuel materials. Specifically, the implications of electronic structure on geometry, thermodynamic stability and electrode potential on one hand and chemical reactivity on the other will be explained.[1-4] Such understanding and insight into the experimentally observed phenomena are particularly valuable when experimental characterization is difficult, being detrimental for nuclear fuel materials for which experimental characterization is rather scarce. Finally, the necessity for careful fine tuning of theoretical methods and models for describing the structure and activity in materials with complex electronic structure will be exemplified.[5]

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