

A Microscopic View of Piezoelectric Oxides

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This talk presents a case study on the application of computer simulations to find new materials for given applications, here transducers. Piezoelectric oxides, particularly certain Pb containing perovskites, are widely used for electro-mechanical transducers, that is, devices that convert sound into electrical energy and vice versa. Applications range from medical ultrasounds to SONAR. In this talk I will overview the physics of these materials and their piezoelectric properties. As will be seen their performance depends on a remarkable balance between different lattice instabilities of the perovskite structure. These in turn depend on the chemistry of Pb, which poses a challenge, because environmental regulations mandate the removal of Pb from electronics. We have been using density functional calculations to understand the details of the lattice instabilities in microscopic terms. This has yielded understanding of how to control them, which is summarized in four design rules as well as a new mechanism for strong ferroelectricity in perovskites.