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CHALLENGES AND OPPORTUNITIES OF FIRST-PRINCIPLES MATERIALS DESIGN

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Abstract. First-principles materials computation involves a group of numerical techniques that allows us to solve fundamental laws of physics and chemistry such as the quantum mechanical Schrödinger equation and Newton's law of motion to tackle problems of technological interest. In recent decades, the availability of important advances in computational software and hardware has enhanced the spectra and complexity of the problems that can be addressed. In addition, as we increase complexity of a given problem, many disciplines (before barely connected) become naturally integrated. All these factors converge to facilitate the understanding of microscopic mechanisms and their relationship to macroscopic properties, and therefore they provide the basis for a first-principles approach to design of materials for specific applications.

Here I would like to highlight a couple of examples showing the challenges and opportunities arising from the proposed approach. Using density functional theory we have been examining new physico-chemical phenomena arising when two metal surfaces approach each other defining a gap of the order of 0.5 nm, right before an "avalanche" mechanism takes the two surfaces to recover the bulk state. Under these conditions, we show that the gap becomes occupied by an electronic cloud able to induce extremely interesting chemical reactions, which go beyond what is usually achieved with a single catalytic surface. [1, 2] We demonstrate the concept showing the evolution of an ethylene molecule under the geometric and electronic confinement, its conversion to a radical anion, and its posterior polymerization without the need of an initiator as in traditional polymerization processes. Further, we examine the electronic and magnetic changes detected on the surfaces. In particular, we explain the changes in magnetic moment as a function of the separation between surfaces and its potential application as sensor devices. The gap-induced phenomena are also important to elucidate corrosion mechanisms in cracks.

References.

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