Atomistic simulations of surface processes in materials for energy production and storage

Rita Magri

Department of Physics, Informatics, and Mathematics, University of Modena and Reggio Emilia, Via G. Campi 213/a, 41125 Modena, Italy

*Corresponding Author E-mail: rita.magri@unimore.it

ABSTRACT

Energy shortage and environmental issues call for the development of clean and sustainable fuel devices and devices for massive energy storage. Recently a great effort has been spent to study new materials to be employed in the next generation electrochemical devices. The main requirement is to design materials for electrodes made up of elements which are not toxic, easy to find on the Earth's crust, not too expensive, easy to recycle, and with a comparable or even better performance than the materials currently in use. Of major importance are also the properties of electrode surfaces and interfaces with polymeric materials (e.g. polymeric binders in batteries). Atomistic simulations are essential to spread light on the material properties not accessible to experiments and on the phenomena taking place on the surfaces and at the interfaces. They can be very helpful in accompanying material development. In this talk I will show our recent progress in the first-principles simulations of electrode materials. Systems, such as metal oxides and silicon anodes, will be addressed, with a particular emphasis for the interaction of silicon with newly proposed [1] binders based on self-healing polymers.

Keywords: Electrodes, Li ion batteries, self-healing, DFT

References:

[1] European Union's Horizon 2020 research and innovation Project Bat4ever "Autonomous Polymer based Self-Healing Components for high performant Li-Ion Batteries"