Computational Modeling Li-ion batteries

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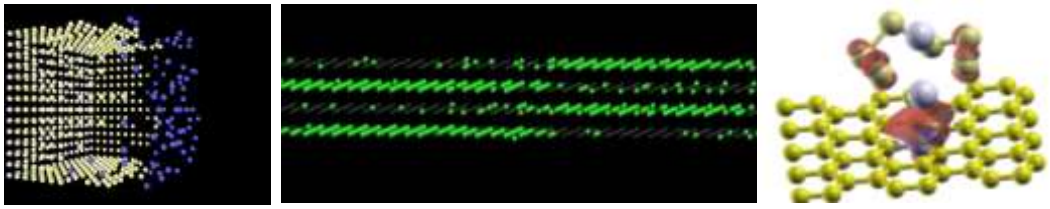
Lithium-ion batteries have allowed to design lightweight accumulators, of small size and varied shapes, with high performance and reliability, specially adapted to the applications of the consumer electronics industry. At first sight, it could appear that the most important properties to consider by these energy accumulation systems are the bulky ones, since Li-ion is stored in many cases in massive materials. However, this phenomenon involves always the transfer of ions and electrons across interphases, so that in many cases kinetic issues are critical to achieve an efficient energy storage.

In the present talk we address, by means of computer simulations, a few Li-ion storage materials in which accounting for interphases and kinetic behavior is essential to understand and tune the performance of these materials.

The figure below illustrates different systems containing Li-ions where interphase effects are important: core-shell formation in anodic materials (a), the occurrence of phase boundaries in graphite (b) and the adsorption of polysulfides on a doped graphite surface.



(a) (b) (c)

Figure: Illustration of Li-ion storage systems where surfaces play a role: (a) formation of a core-shell structure simulated by kinetic Monte Carlo (KMC). Blue: Li^+ diffusing ions, yellow: deposited Li^+ ions, white: metallic contact; (b) occurrence of a phase boundary for Li^+ insertion in graphite, as simulated by KMC. Green spheres denote Li^+ ions; (c) Adsorption of a L_2S_6 polysulfide on a graphene surface doped with a B atom.