# Simulations of carbon-based electrodes for a new generation of more efficient bateries

**Researchers:**

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Idioma Indefinido

**Descrição:**

Proyecto asignado a través de la Red Española de Supercomputación (RES [2]).

Solid state batteries have recently acquired a great importance due to their advantages respect the other types. Normally, graphite has been chosen as the anode electrode due to the fantastic electronic properties and the low chemical reactivity. Doping the C-based structures with N, an improvement in the electrode performance is obtained. In this project, using precise mechano-quantum calculations based on the Density Functional Theory, we have planned to study graphite and nanotubes doped with different elements (N or B) in order to establish their potential improvement in the electronic interchange as well as the ionic mobility. We will study the inclusion of different types and number of alkaline ions (Li, Na, K) to find the best arrangements and the saturation number. All these parameters will suggest the best future electrode.



**Ligações**

[1] http://www.ucm.es/ [2] https://www.res.es/