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"In Silico" Design of Novel Materials for the Next Generation of Lithium Batteries

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The specific storage capacity of current rechargeable lithium batteries represents a serious limitation for their use in applications such as electric vehicles. One of the most promising technologies for the next generation of Li batteries are rechargeable lithium-sulfur (Li-S) batteries [1-5]. These are based on a cathode of a sulfur composite, an organic electrolyte and metallic lithium as the active material for the anode. However, the implementation of Li-S batteries in everyday applications still presents several technical drawbacks that must yet be overcome.

Most notably, the so-called "shuttle effect", originated by the migration of Li_2S_x (x = 2, 4, 6, 8) species on the side of the cathode; the generation of lithium dendrites on the side of the anode, are only two of the most prominent problems that have not yet met a definite solution.

One possible solution for both of these problems is the use of laminar 2D materials, such functionalized graphene sheets, or doped graphitic carbon nitride [6].

In this work, we show how ab initio computational modeling at the DFT level can be used as a very useful tool to guide the design of tailored-made surfaces with specific electronic properties to address on one hand the adsorption and electrocatalysis of lithium polysulfides in the cathode, and on the other hand, to provide multiple sites for lithium nucleation and low diffusion barriers for a more homogeneous patting process in the anode.

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