Graphyne as a material for energy storage: a DFT investigation

Nicola Seriani

The Abdus Salam ICTP, Strada Costiera 11, 34151 Trieste, Italy)

nseriani@ictp.it

Abstract

We have investigated properties of the carbon-allotrope graphyne, in view of a possible employment in energy storage, by density functional theory. Bilayers of graphyne and its boron nitride derivatives display a promising behaviour as nanocapacitors, superior to those of graphene and boron nitride. Concerning battery applications, the adsorption of sodium on graphyne has been considered. Sodium adsorption is endothermic, and therefore likely to result in sodium aggregation rather than intercalation. This makes graphyne not a suitable anode material for sodium batteries. I will critically discuss the potential of graphyne for applications, and the challenges ahead.

References

[1] B. Bhattacharya, U. Sarkar, N. Seriani, The Journal of Physical Chemistry C, 120 (2016), 26579.

[2] U. Sarkar, B. Bhattacharya, N. Seriani, Chemical Physics, 461 (2015), 74.

Figures

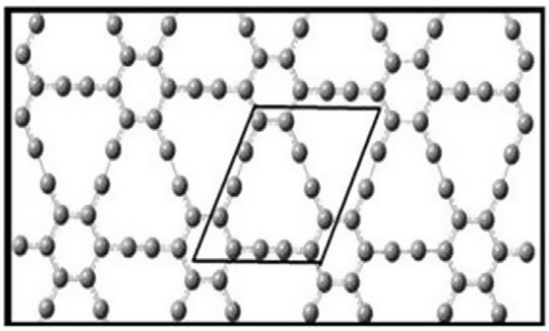

Figure 1: Atomic structure of graphyne

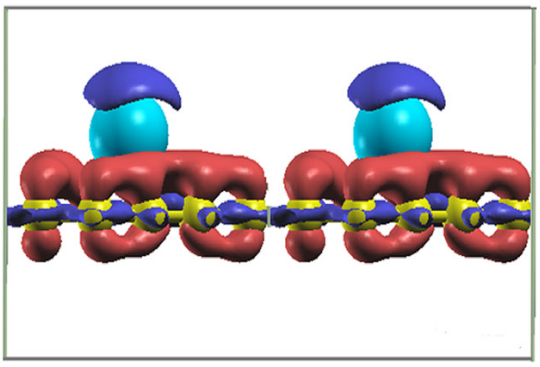

Figure 2: Charge donation from sodium to graphyne. Red indicates charge accumulation, blue indicates charge loss.