# NOVEL NANO-POROUS GRAPHITES FOR GAS STORAGE AND RELEASE

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Pristine graphene is in principle an ideal adsorbing material due to its large specific area, stability, mechanical properties and low weight. Nevertheless, the physisorption of light gas species on graphene is in general not particularly favourable, being the adsorption energy, mainly determined by van der Waals interactions, not large enough to guarantee significant storage capacities at standard temperature and pressure. Intercalation between graphene layers could lead to more encouraging adsorption energies but, unfortunately, in pure graphite there is no room for any atomic or molecular species to be hosted.

A possible solution to this problem is the use of porous derivative of graphene as "building blocks" to construct a new class of porous graphites characterized by a larger interlayer volume available for gas storage. To this regard graphynes, which are novel two-dimensional (2D) carbon-based materials, represent promising candidates since they naturally exhibit a nanoweb-like structure characterized by triangular and regularly distributed subnanometer pores[1]. These intriguing features make them appealing for molecular filtering as shown by recent theoretical predictions[2].

The possibility to exploit graphynes as ideal media for the reversible storage of light gases is here theoretically investigated. The focus is first on molecular hydrogen ($H_2$) and, by means of computations at the MP2C[3] level of theory, it is found that graphynes are more suited than graphene for gas hosting since they provide larger binding energies at equilibrium distances much closer to the 2D plane. In particular, for graphtriyne a flat minimum located right in the geometric center of the pore is identified. A novel graphite composed of graphtriyne stacked sheets is then proposed[4] and an estimation of its 3D arrangement is obtained at the DFT (plus dispersion corrections) level of theory by considering a periodic model of the involved bilayers. In contrast to pristine graphite, this new carbon material allow both $H_2$ intercalation and out-of-plane diffusion and related binding energies are obtained by means of MP2C computations: they are found to almost double the estimation for the adsorption on graphene and they could lead to high $H_2$ storage capacities exceeding those found to date for carbon nanostructures of different nature. The proposed layered carbon allotrope also show a preferential adsorption of carbon dioxide ($CO_2$) with respect to other major components ($N_2$, $H_2O$) of the earth atmosphere and could be postulated as an efficient medium for $CO_2$ separation and capture.

## References

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