STRUCTURAL, ELECTRONIC AND MECHANICAL PROPERTIES OF MOLECULARLY PILLARED 3D NANOPOROUS GRAPHENE MATERIALS.

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ABSTRACT

Molecularly Pillared Nanoporous Graphene materials consist a new category of microporous materials in which graphene sheets are separated as a result of intercalation of organic molecules. The intercalated organic molecules act as spacers between the graphene sheets with which they are attached via covalently bonded and judiciously chosen linking moieties. These materials are candidates for a variety of applications with primary targets in flexible electronics, photovoltaics, gas separation and sensing and photocatalysis. A feature of these materials of central importance is the ability they offer for tuning their electromechanical properties by variation of several structural parameters such as linker size, in-layer linker distribution, intra-layer relative linker density and the chosen functionalization of the organic linkers.

The molecular structure and the electronic and mechanical properties of the proposed pillared graphene materials have been studied by systematically varying the chemical type, the linker density, the linker distribution and performing electronic structure computations and molecular mechanics simulations. The results reveal that the pillar density and their distribution between the graphene sheets have a stronger effect on the electronic properties compared to substitution of pillars with others of different chemical type, for those that were considered. This allows tuning the energy gap these materials making them from semiconducting to metallic. Moreover, we show that the calculated elastic moduli of the proposed materials can be reduced by decreasing the size of the organic linker or by increasing the linker density.