Disordered Graphene Materials: Atomistic Characterization and Performances

Aleandro Antidormi[1]
Stephan Roche[1,2]
[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193, Barcelona, Spain*
[2] *ICREA Institucio Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain*
aleandro.antidormi@icn2.cat

Formidable progress has been recently achieved in the fabrication and characterization of disordered materials with unprecedented properties. In this context, particular forms of disordered graphene (reduced graphene oxides), obtained by chemical exfoliation techniques, have been found suitable to improve the performances of composite materials, with application in energy. Moreover, the recent demonstrated possibility to synthesize wafer-scale two-dimensional amorphous carbon monolayers, structurally dominated by sp2 hybridization has initiated a new platform of low-dimensional materials to explore as alternative forms of membranes with enhanced chemical reactivity which could serve as coating materials [1,2].
The excellent physical properties of the mentioned materials derive from the nature and degree of their disorder which, controlled at the fabrication level, represents the key ingredient to tune their physical/chemical properties for specific target applications. In this respect, new fabrication strategies to modify the degree of disorder and a systematic theoretical characterization of the impact of the material structural quality on the ultimate performance is urgent.
In this poster we present the results of our theoretical investigation on possible strategies to improve the (thermal) reduction process of graphene-oxides and the consequent possibility to recover the quality of pristine graphene [3]. Moreover, we present a systematic analysis of the structural and vibrational properties of amorphous carbon monolayers as a function of the structural quality of the material, showing how disorder results in a tunable thermal conductivity varying by more than one order of magnitude [4]. In particular, we identify how energy is dissipated in this material by a systematic analysis of emerging vibrational modes whose localization increases with the loss of spatial symmetries. Our simulations provide some recipe to design most suitable "amorphous graphene" based on the target applications such as ultrathin heat spreaders, energy harvesters or insulating thermal barriers.

REFERENCES

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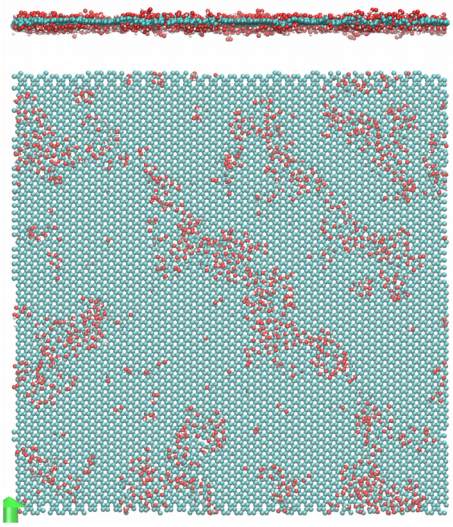

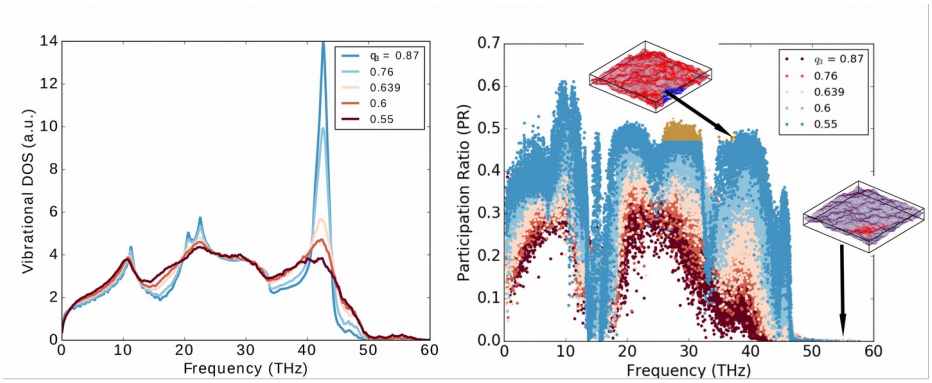

FIGURES
Figure 1: Side and top view of a GO sample before thermal reduction.
Figure 2: (Left) Vibrational DOS of Amorhous Graphene for different degrees of amorphousness. (Right) Participation Ratio of the samples and atomic displacements (insets)