University of Crete
Department of Physics

Physics Colloquium

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Modeling 2D materials and biomolecular systems

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ABSTRACT

I discuss a number of results obtained over the last years on two-dimensional materials and systems of biological interest.

In the former case, I present a numerical method to compute the phonon dispersion of these materials and the dependence on temperature or mechanical strain. Applications in graphene and hexagonal boron nitride will be considered. Then, I switch to mechanical response and in particular in the uniaxial compression and buckling of graphene and graphene nanoribbons.

In the latter case, various properties of DNA will be discussed, including base-pair thermal openings and possible connections to biological function, as well as charge transfer rates between properly engineered donor and acceptor sites within the biomolecule.