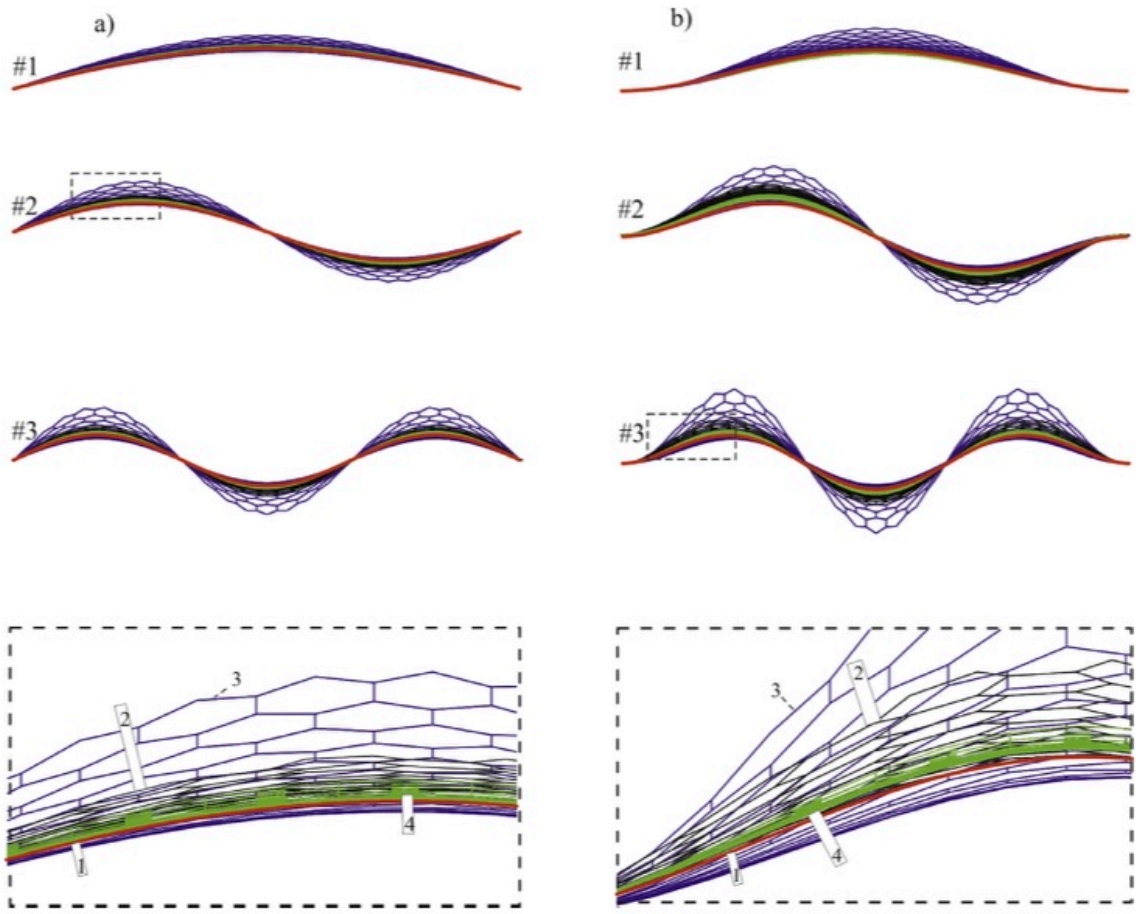
The Molecular Mechanics of Single Layer Graphene Sheets

S.N. Korobeynikov

Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia



Molecular mechanics (MM) method is widely used to simulate the deformation, vibration and buckling of sp2 carbon nanoforms. The MM method can be divided into the standard MM method, based on the direct use of atomic interaction force fields, and the molecular structural mechanics (MSM) method for the problems of deformation, vibration, and buckling of sp2 carbon nanoforms. In the MSM method potential energies of bonded and non-bonded atomic interactions are approximated by potential energies of beam and truss elements. The MM and MSM methods allow to model the mechanical moduli of graphene. In the latter case, it is important to use parameters of force fields and beam elements that most accurately reproduce these mechanical moduli.

The present study has the following objectives: (1) to modify the parameter set of the DREIDING force field in order to improve the agreement between the simulated mechanical moduli of graphene and the their reference values for this material; (2) to develop a new approach to determine the set of geometric and material parameters for a Bernoulli-Euler beam element with a circular cross-section that provides an accurate reproduction of reference values of 2D Young's modulus, Poisson's ratio, and bending rigidity modulus of graphene; (3) to perform a comparative analysis of the free vibration frequencies and modes of SLGSs obtained by both (standard MM and MSM) methods by means of computer simulations using the PIONER and MSC.Marc codes.

Mercoledí 15 Maggio 2019, ore 15:00
via della Madonna dei Monti, 40 - Aula De Vecchi

Università Roma Tre – Dipartimento di Architettura
Laboratorio Interdipartimentale di Matematica Applicata e Meccanica delle Strutture (LIMeS)