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The Non Linear Behaviour of Carbon Based Nanostructures: A Molecular Mechanics Model

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From about twenty years carbon-based nanostructures are a real challenge for the scientific community, for their enormous technological potential in several contexts of application, including microelectronics (e.g., conductive inks and flexible films), sensoring and actuating systems (e.g., gas sensors), energy generation and storage (e.g., photovoltaic cells, hydrogen storage, supercapacitors), biotechnologies (e.g., membranes for water filtration, gas separation, DNA sequencing) and composites [1-5]. Their effective exploitation goes hand in hand with in-depth knowledge of their physical behavior. Electronic, optical and mechanics properties are crucial and, moreover, also mutually interacting, even with the possibility of tuning the former trough control of deformation. Knowledge of the mechanical behavior of these nanostructures is also related to the availability of predictive models, e.g., provided by ab-initio methods [6], by molecular dynamics (or statics) [7-8], but also by continuum mechanics [9] and structural mechanics [10]. In the context of linearized models, aimed at determining the elastic moduli, the cost of computationally onerous methods is not prohibitive; on the contrary, when the mechanical behaviour is highly non-linear, e.g., in post-buckling behaviour, in case of mode interaction or in fracture problems, the recourse to models as simple as possible is necessary. In the present paper a molecular mechanics model, equipped by simple potentials, incorporating binary, ternary and quaternary atomic interactions, is presented and the choice of the parameters of the given potentials is explained. The model is implemented in a numerical algorithm of step-by-step analysis with the objective to provide the equilibrium paths also in advanced post-buckling. Both the accuracy of the model and the reliability of the implementation are valued by means of a tight comparison with results in the literature of Solids State Physics.

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