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A method for efficient structural simulation of carbon nanostructures and its application to irradiated graphene nanoribbons COLIN DANIELS, ZACHARY BULLARD, Rensselaer Polytech Inst, EDUARDO COSTA GIRÃO, Universidade Federal do Piauí, VINCENT MEUNIER, Rensselaer Polytech Inst — Graphene based nanostructures, including defective ones, are of particular interest for many applications. Due to the inherent stochastic nature of defects in real structures, traditional molecular dynamics approaches are ill-suited for examining average behaviors over time scales relevant to realistic experimental conditions. This talk will introduce and discuss the results of the application of an original Monte-Carlo algorithm for the efficient simulation of the time evolution of carbon nanostructures as they are exposed to external stimuli. I will begin with an overview of the algorithm used, including some simple examples, and move on to an in-depth examination of the application of this algorithm to graphene nanoribbons. In particular, I will examine the atomistic restructuring of different types of carbon nanoribbons as they are irradiated and subjected to uniaxial stress, and discuss the novel properties that emerged thereof. Additionally, the examination will shed light on the use of this method in practice and highlight the utility of other methods, used in conjunction with this algorithm, that allowed for fast prototyping of the system's electronic and magnetic properties.

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