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**Some lessons learned on the simulation of atomic-scale stochastic processes in carbon systems** VINCENT MEUNIER, COLIN DANIELS, ZACHARY BULLARD, Rensselaer Polytechnic Institute, ICMP TEAM — The behaviors of many materials are rooted in stochastic processes due to spatial and temporal fluctuations in their nano- and micro- structures. This talk will be the opportunity to present preliminary results on attempts to shed light on the role played by disorder on the dynamical appearance of atomic-scale defects and how these build their way up to mesoscopic length scales and over macroscopic time scales. I will present a simple algorithm that allows translating atomic level properties into scales relevant to devices and materials systems. The algorithm enables the random introduction of elementary mutations in low-dimensional systems and leads to the investigation of the emergence of structures with new functionality and to novel nanostructures resulting from the coalescence of elementary building blocks. The mutations are introduced by local modifications to the connectivity table and are accepted based on a Metropolis algorithm. Externally imposed constraints can be introduced as needed, depending on the actual conditions to be simulated. In addition, the fast prototyping of the effect of mutations on electronic properties is made possible by the ability to enact mutations as perturbation potentials using Dyson equation to update Green functions as mutations are accepted. Results applied to the coalescence, annealing, and phase separation in a number of carbon nanostructures will be shown and compared to experiments when available.

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