Abstract Submitted
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Structural modeling of amorphous graphene: a differential-mutation approach KATJA BISWAS, University of North Georgia — A modified differential-mutation algorithm will be presented that can reliably produce low-lying energy structures of amorphous systems. The algorithm merges a genetic algorithm with a computational cooling procedure. This makes it possible to obtain low-lying energy minima with a very limited population size. The algorithm has been implemented for structural optimization of amorphous graphene, where the individual carbon atoms interact via a classical bond-order potential. It will be shown that the resulting minimum configurations are very close in energy and represent locally different topological structures of the material. The results for the coordination numbers, ring-size distribution and puckering of the amorphous surface will be discussed.

Katja Biswas
The University of North Georgia

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