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A proposed method for directed self-assembly of graphene nanoribbons JAMES GERAETS, REIDUN TWAROCK, YVETTE HANCOCK, University of York — There is an opportunity for modeling to inform the experimental synthesis and design of graphene nanoribbons (GNRs). We present here a new course-grained algorithm for simulating GNR synthesis by the self-assembly of aromatic carbon precursor molecules. The model uses a Gillespie algorithm to form a network of possible coupling reactions between these molecules, and exploits a novel way of representing their geometries to speed up the simulations. Based on this method, we identify areas in parameter space given by temperature, binding energy, functional groups, and concentration of precursor molecules, which lead to GNRs with desirable properties. We demonstrate use of the model based on two precursors that self-assemble together to form a nanoporous GNR, namely, functionalized tetrabenzanthracene and benzene. We demonstrate that, unlike a pristine GNR, the GNRs formed by these molecules have regular repeating holes, and exhibit a band gap of 1.6eV independent of the ribbon width.

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