Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Theory of pore-edge interactions and resulting patterns in graphene nanoribbons LIN DU, LIN HU, University of Massachusetts Amherst, ANDRE MUNIZ, Federal University of Rio Grande do Sul, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We report a systematic analysis of pore-edge interactions in graphene nanoribbons (GNRs) and their outcomes based on first-principles calculations and atomic-scale simulations according to reliable interatomic potentials. Energetic computations reveal strongly attractive interactions when the edge of a nanopore (vacancy cluster) in the GNR and a GNR edge are in close proximity to each other. We derive functional forms for these interaction potentials and characterize the effects of pore size and GNR edge type on these interactions. We conduct molecular-dynamics (MD) simulations of nanopore dynamics at high temperature for nanopores in the vicinity of GNR edges under the thermodynamic driving force for nanopore migration provided by the attractive pore-edge interactions. We find that pore migration toward the GNR edge is mediated by a sequence of carbon ring reconstructions, which cause pore coalescence with the GNR edge. Subsequent morphological evolution of the GNR edge leads to edge pattern formation, controlled by the pore size and the GNR edge type. We construct the underlying optimal kinetic pathways through nudged-elastic-band calculations and characterize the electronic structure of the resulting GNRs with patterned edges.

Lin Du
University of Massachusetts Amherst

Date submitted: 07 Nov 2016 Electronic form version 1.4