Title: Molecular dynamics study of graphene Moebius bands: equilibrium shapes and energies

Name: Yoichi Takato and Eliot Fried
Okinawa Institute of Science and Technology Graduate University
1919-1 Tancha, Onna-son, Kunigami-gun, Okinawa, Japan 904-0495

Graphene is a highly flexible 2D material that can easily bend and fold. This mechanical flexibility allows us to build various graphene-based structures such as carbon nanotubes and nano-origami shapes. The Moebius band, a non-orientable one-sided surface constructed by twisting a rectangular strip by 180 degrees and joining the ends, is a theoretically possible graphene-based structure but has not yet been observed in the laboratory. We use molecular dynamics to determine the equilibrium shapes and mechanical energies of Moebius bands made of monolayer graphene nanoribbons with armchair and zigzag edges. Our results show resemblance to continuum Moebius bands regardless of the discrete nature of the lattice structure and associated edge types. From the structural stability and energetics views, we discuss the feasibility of fabricating nanoscale graphene Moebius bands.

Presenting author details
Full name: Yoichi Takato
Contact number:
Twitter account: yoichi_tak
Linked In account: www.linkedin.com/in/yoichi-takato-70848378
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