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Molecular dynamics study of graphene mobius bands: Equilibrium shapes and energies**Yoichi Takato and Eliot Fried**

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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 Mobius 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 Mobius bands made of monolayer graphene nanoribbons with armchair and zigzag edges. Our results show resemblance to continuum Mobius 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 Mobius bands.

Biography

Yoichi Takato is presently associated with Okinawa Institute of Science and Technology, Japan. He has published numerous research papers and articles in reputed journals and has various other achievements in the related studies. He has extended his valuable service towards the scientific community with his extensive research work.

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