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Electromechanical Characterization of Carbon Nanotubes in Torsion via Symmetry-Adapted Tight-Binding Objective Molecular Dynamics DONG-BO ZHANG, TRAIAN DUMITRICA, RICHARD JAMES, University of Minnesota — The nonlinear elastic response of carbon nanotubes (CNTs) in torsion is derived with objective molecular dynamics and a density-functional-based tight-binding model. The critical strain beyond which CNTs behave nonlinearly, the most favorable rippling morphology, and the twist- and morphology-related changes in fundamental band gap are identified from a rigorous atomistic description. There is a sharply contrasting behavior in the electronic response: While in single-walled CNTs the band gap variations are dominated by rippling, multi-walled CNTs exhibit an unexpected insensitivity. Results are assistive for experiments performed on CNT-pedal devices. References: D.B. Zhang, R.D. James, and T. Dumitrica, "Electromechanical Characterization of Carbon Nanotubes in Torsion via Symmetry-Adapted Tight-Binding Objective Molecular Dynamics," Physical Review B 80, 115418 (2009).

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