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Helical Nanotube Structures of MoS2 with Intrinsic Twisting: An Objective Molecular Dynamics Study TRAIAN DUMITRICA, DONG-BO ZHANG, University of Minnesota, GOTTHARD SEIFERT, Technische Universitaet Dresden — Objective molecular dynamics combined with density-functional-based tight-binding makes possible to compute chiral nanotubes as axial-screw dislocations. This methodology enables the surprising revelation of a large catalog of MoS_2 nanotubes that lack the prescribed translational symmetry and exhibit chirality-dependent electronic band-gaps and elastic constants. Helical symmetry emerges as the natural property to rely on when studying quasi-one dimensional nanomaterials formally derived or grown via screw dislocations.

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