

Abstract Submitted  
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**Helical Nanotube Structures of MoS<sub>2</sub> with Intrinsic Twisting:  
An Objective Molecular Dynamics Study** TRAIAN DUMITRICA, DONG-BO  
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Dresden — Objective molecular dynamics combined with density-functional-based  
tight-binding makes possible to compute chiral nanotubes as axial-screw disloca-  
tions. This methodology enables the surprising revelation of a large catalog of MoS<sub>2</sub>  
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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