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Screw Dislocated ZnO and Si Nanostructures Studied with Objective Molecular Dynamics EVGENIYA AKATYEVA, ILIA NIKIFOROV, DONG-BO ZHANG, TRAIAN DUMITRICA, University of Minnesota — Objective molecular dynamics [1] coupled with tight-binding density functional-based models makes it possible to investigate the stability and electronic structure of ZnO and Si nanotubes [2] and nanowires [3] containing axial screw dislocations. The dislocated structures adopt twisted configurations that stabilize the dislocation at the center despite the close vicinity of surfaces, in excellent agreement with Eshelby's elasticity model of cylinders containing an axial screw dislocation. Coupled to this elasticity model, our simulations represent a new efficient method of calculating the core energy of a dislocation and allow to rationalize the stability of chiral hollow nanowires. The uncovered mechanical and electronic behaviors have implications for a broad class of nanomaterials grown by engaging a screw dislocation. 1. T. Dumitrica and R.D. James, J. Mech. Phys. Sol. 55, 2206-2236 (2007). 2. D.-B. Zhang, E. Akatyeva, and T. Dumitrica, Phys. Rev. B 84, 115431 (2011). 3. I. Nikiforov, D.-B. Zhang, and T. Dumitrica, J. Phys. Chem. Lett. 2, 2544 (2011).

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