Abstract Submitted
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Quantum Simulations of One-Dimensional Nanostructures under Arbitrary Deformations[1] PEKKA KOSKINEN, University of Jyvaskyla — A powerful technique is discussed for simulating mechanical and electromechanical properties of one-dimensional nanostructures under arbitrary combinations of bending, twisting, and stretching.[1] The technique is based on an unconventional control of periodic symmetry[2], which eliminates artifacts due to deformation constraints and quantum finite-size effects and allows transparent electronic-structure analysis. Via density-functional tight-binding implementation, the technique demonstrates nonlinear electromechanical properties in carbon nanotubes and abrupt behavior in the structural yielding of Au_7 and Mo_6S_6 nanowires. The technique drives simulations closer to more realistic modeling of slender one-dimensional nanostructures under experimental conditions. [1] P. Koskinen Phys. Rev. Applied 6, 034014 (2016)
[2] P. Koskinen and O. O. Kit Phys. Rev. Lett. 105, 106401 (2010)

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