

Electronic properties of twisted MoS₂-nanotubes

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During the last years, intensive research has been done on electronic properties of inorganic nanotubes (INT) built by metal dichalcogenides. They possess desirable intrinsic band gaps and intrinsic stick-slip behavior (1) indicating their potential for nanoelectromechanical devices.

Here, we present a theoretical study on the electronic properties of MoS₂-nanotubes suspended to mechanical strain and torsion. To minimize computational cost, we performed DFTB (2) calculation with helical boundary conditions (3) allowing us to choose the size of the unit cell independent from the applied twist angle, although the initial translational symmetry is broken. We show that twisting an MoS₂-nanotube leads to a decrease in the energy gap and therefore an increase in conductivity, following the phenomenological transport model. Our calculations are verified through experimental studies on twisted INTs exhibiting a highly repeatable response to torsion and strain.(4)

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