Electromechanics in MoS_2 and WS_2: nanotubes vs. monolayers

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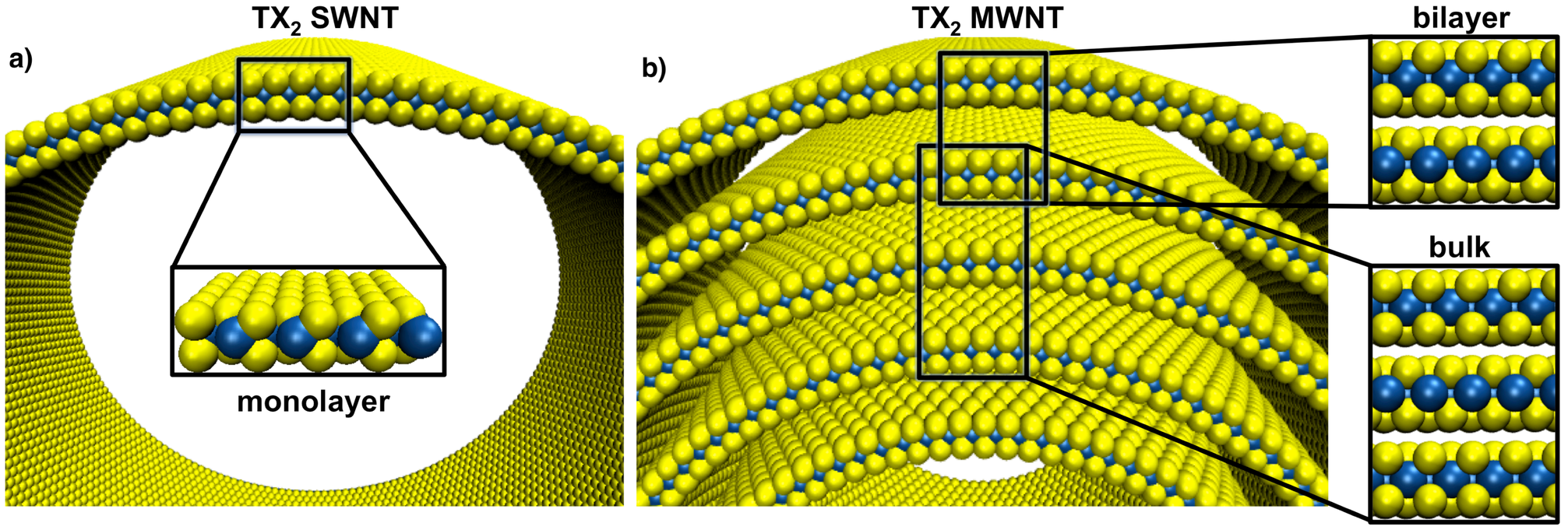
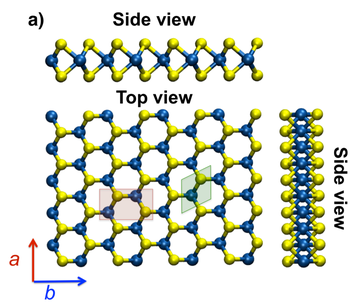
Abstract

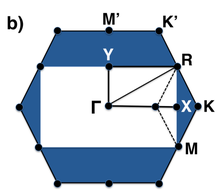
The transition metal dichalcogenides (TMD) MoS_2 and WS_2 show remarkable electromechanical properties. Strain modifies the direct band gap into an indirect one, and substantial strain even induces an semiconductor-metal transition. Providing strain through mechanical contacts is difficult for TMD monolayers, but state-of-the-art for TMD nanotubes. We show using density-functional theory that similar electromechanical properties as in monolayer and bulk TMDs are found for large diameter TMD single (SWNT)- and multi-walled nanotubes (MWNTs). The semiconductor-metal transition occurs at elongations of 16%. We show that Raman spectroscopy is an excellent tool to determine the strain of the nanotubes and hence monitor the progress of that nanoelectromechanical experiment in situ. TMD MWNTs show twice the electric conductance compared to SWNTs, and each wall of the MWNTs contributes to the conductance proportional to its diameter.

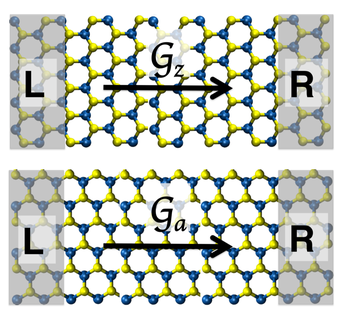


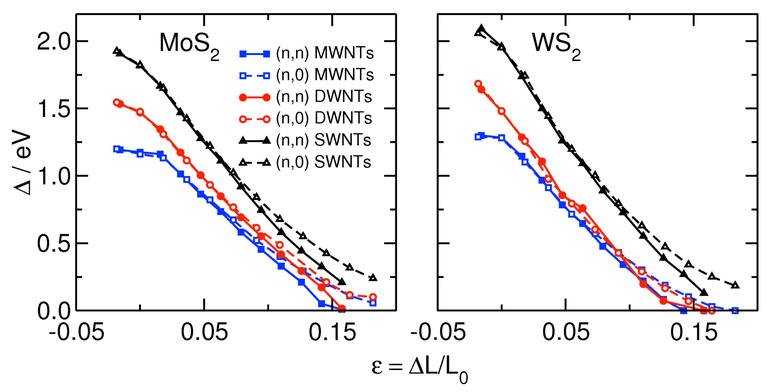
Electronic Structure

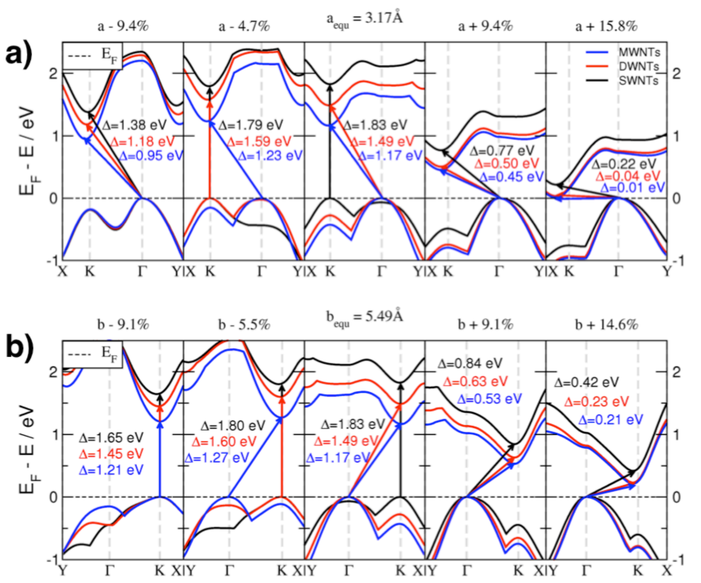
- Slight mechanical deformation of the SWNTs would result in a change of the direct band gap back to the indirect one.
- A general property is that tensile strain (ε) linearly reduces Δ. Further stretching results in a semiconductor-metal transition.



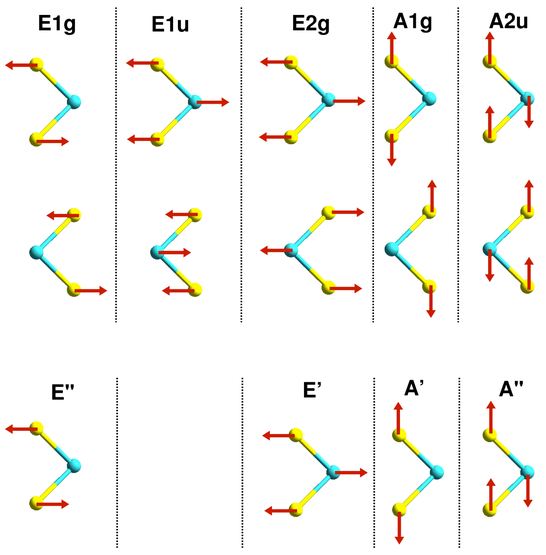








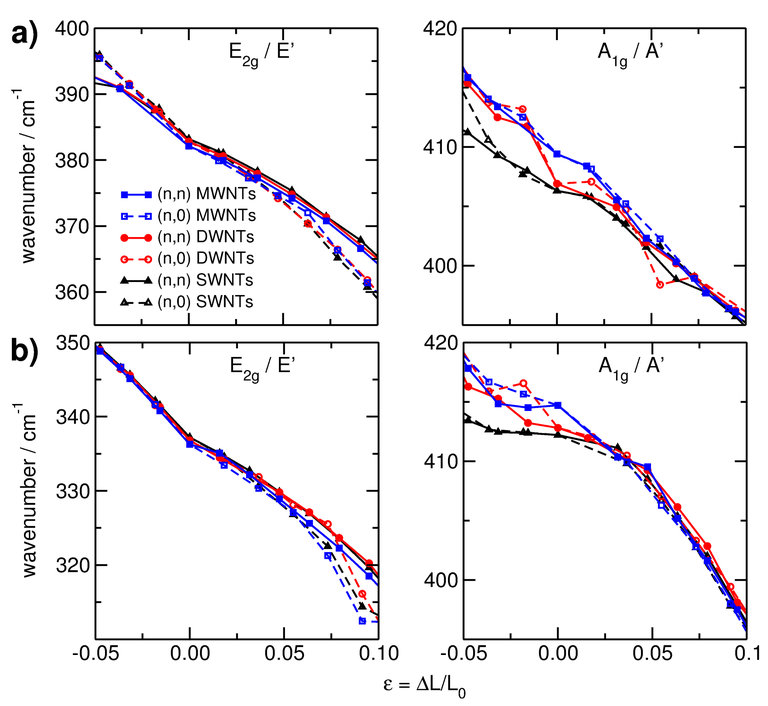
Lattice Dynamics

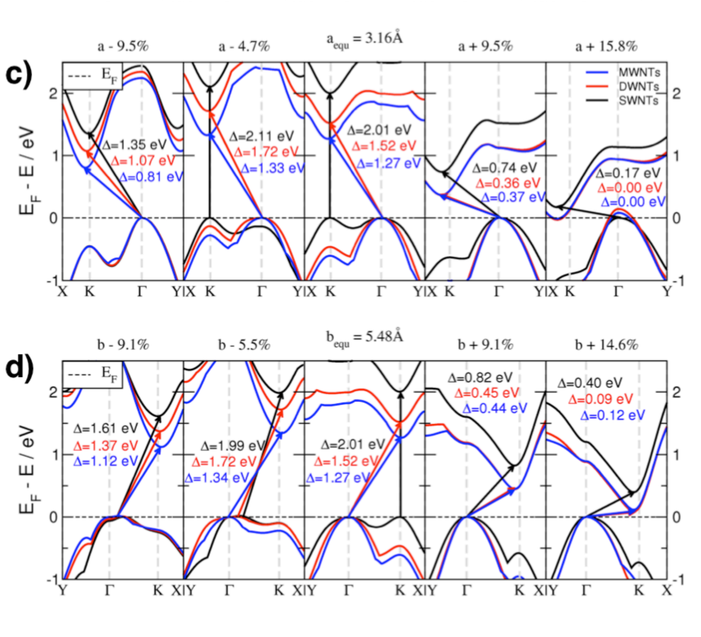


Bulk / Multilayer

Quantum confinement 3D➔2D slightly changes lattice dynamics: A_{1g} becomes softer, transforming into the A′, while E_{2g} harden, transforming into the E′.

Monolayer

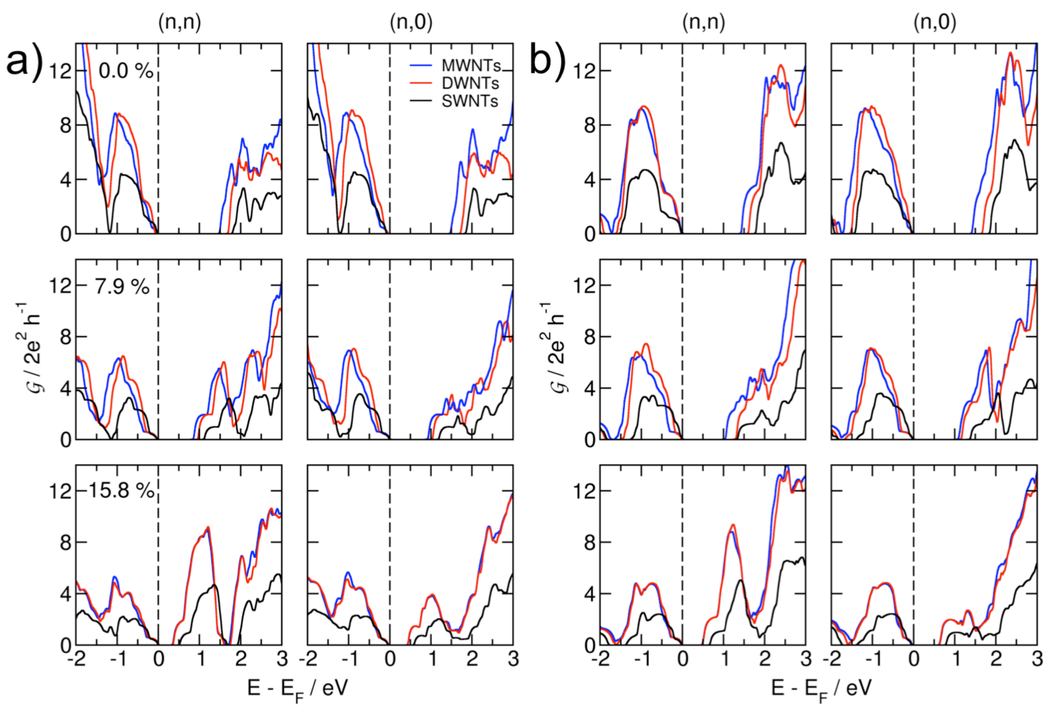




- Mechanical deformations strongly alter the lattice dynamics: frequencies change almost linear over a long range of elongations and similarly for different chiralities up to a strain of ~8 %.

Quantum Transport

- As TMDs are stretched along tube axis, conductance appears closer to the Fermi level and eventually transport channel opens.



Theoretical Methods

- DFT/PBE as implemented in Crystal09 with all-electron 86-311G* basis for S and effective core potential approach with large cores for Mo/W, accounting for scalar relativistic effects.
- The coherent electronic transport calculations were carried out using density functional based tight-binding (DFTB) method in conjunction with the Green's function technique and the Landauer-Büttiker approach.

Conclusions

- Large-diameter NTs can be approximated with layered systems as their properties should be nearly the same at the scale.
- Electronic properties of TMD NTs and layers can be controlled by an external tensile strain for nanoelectromechanical applications.
- Raman spectroscopy is an excellent tool to monitor the effect of strain in the samples.

References

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Acknowledgments

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