Modulation of electron transport in single layer transition-metal dichalcogenides

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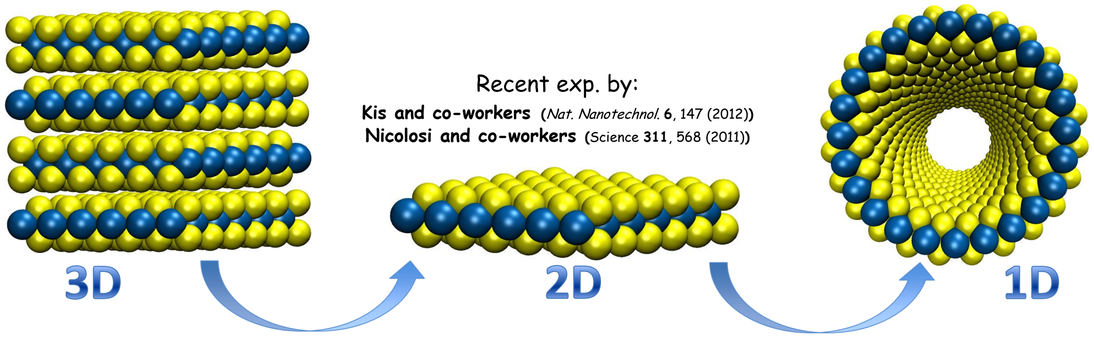
Abstract

Transition-metal dichalcogenides TX_2 (T=Mo, Nb, Ta, Re, Hf, W and X=Se, S, Te) may become alternatives to carbon based materials in nano-electronics. Recently, a series of electronic devices have been fabricated using a single layer of MoS_2, presenting promising potential for the next generation electronics. Using density functional based tight-binding (DFTB) method combined with the non-equilibrium Green's function formalism, we have studied electron transport in low-dimensional structures of transition-metal dichalgogenides.

Exp. literature well-known for last **40 years**

Recent exp. by:
Kis and co-workers (*Nat. Nanotechnol.* **6**, 147 (2012))
Nicolosi and co-workers (Science **311**, 568 (2011))

Exp. known since 1992:
Tenne and co-workers (*Nature* **360**, 444 (1992))



Formalism

Green's function of an extended system

$$\tilde{G}_C(E) = \left[ES_C - H_C - \tilde{S}_L(E) - \tilde{S}_R(E) \right]^{-1} \qquad \tilde{\Gamma}_{L(R)} = i[\tilde{S}_{L(R)} - \tilde{S}^{+}_{L(R)}]$$

DFTB

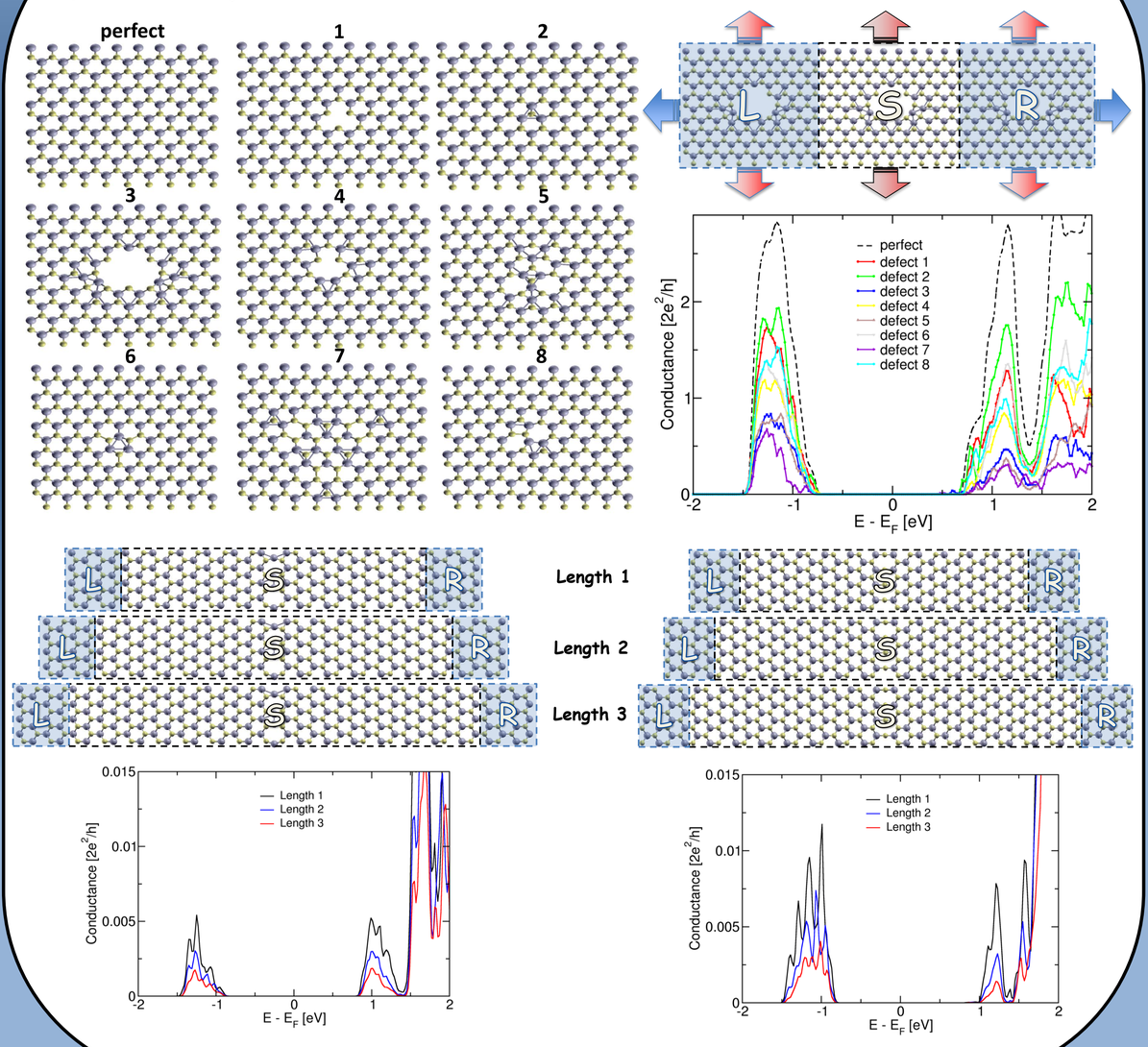
Transmission

$$T(E) = \sum_n T_n(E) = Tr\left[\tilde{G}^{\dagger}_C(E)\tilde{\Gamma}_R(E)\tilde{G}_C(E)\tilde{\Gamma}_L(E) \right]$$

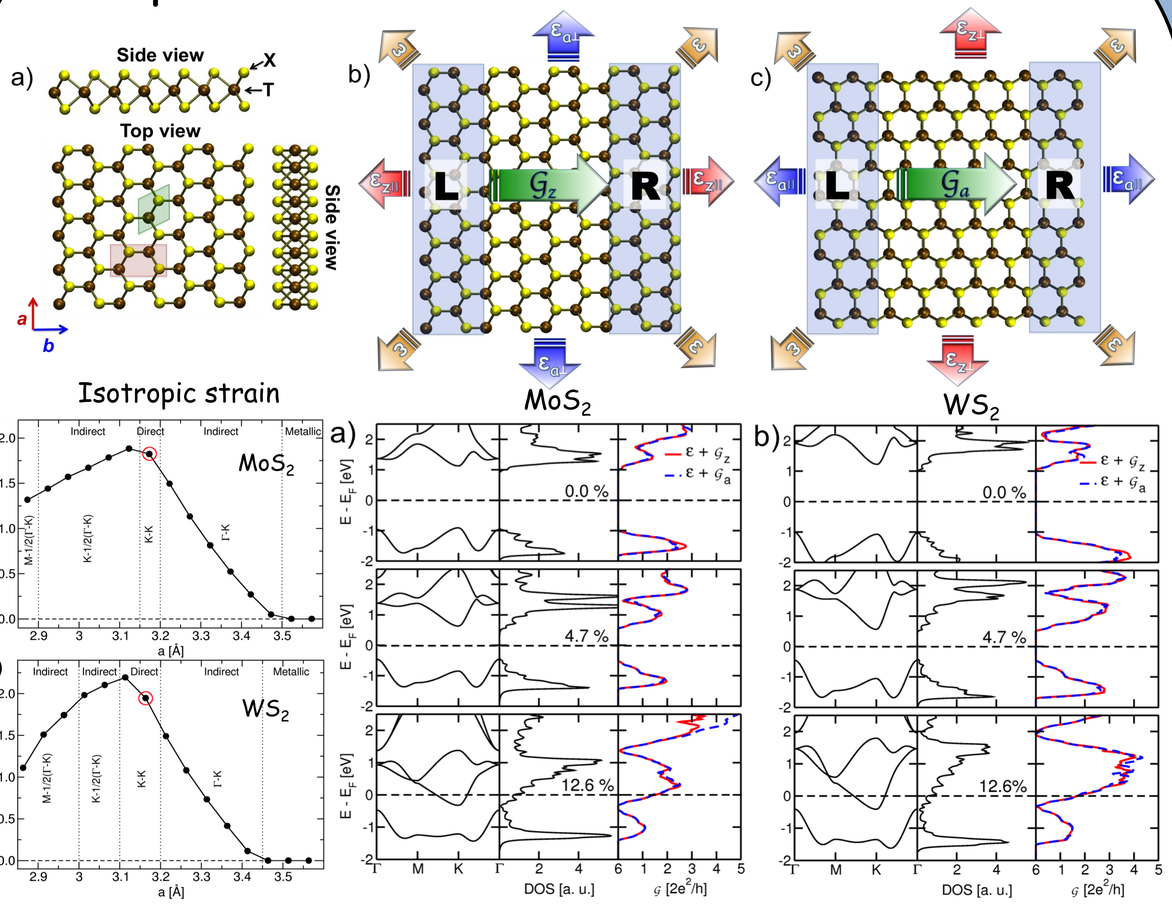
Conductance

$$\mathcal{G}(E) = \frac{2e^2}{h} T(E)$$

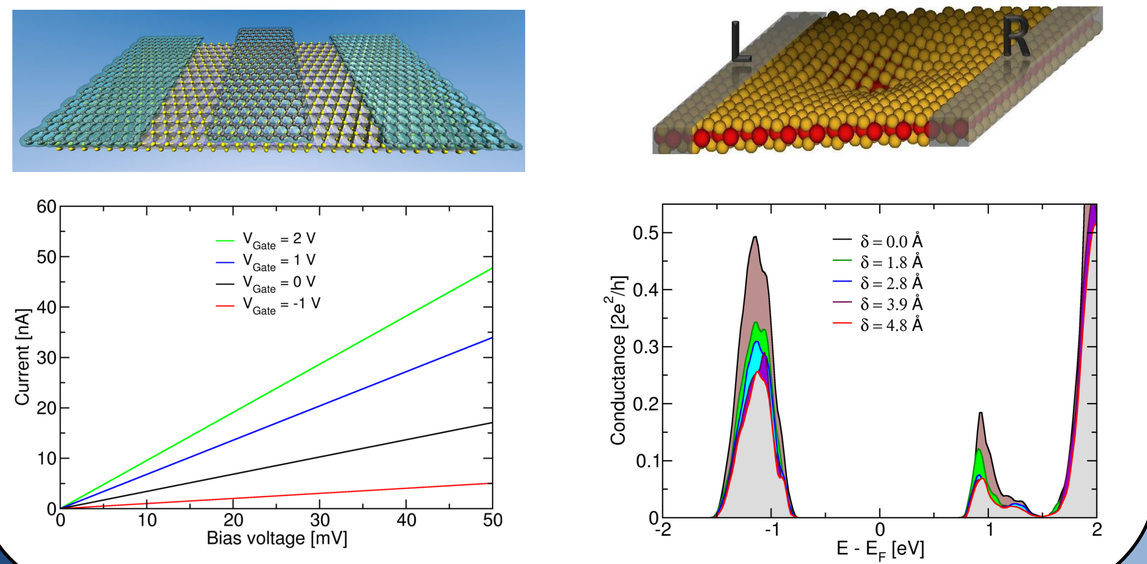
Local defects



Isotropic and uni-axial strain



Graphene and MoS_2



Nano-indentation

Conclusion

- Local defects cause reduction of conductance in MoS_2 monolayer, while the band gap changes only slightly.
- The use of graphene as a metallic electrode for MoS_2 monolayer shows efficient electron injection and ohmic contact through Graphene/MoS_2/Graphene junction.
- Tensile strain is a possible way of tuning the band gaps and transport properties of TMD monolayers. The transition semiconductor-metal occurs for elongations as large as 11% for the isotropic strain in MoS_2 monolayer .
- Local deformation due to the indentation process causes a drop of electron conductance, in our model to 60% of its original value. Thus, the electronic structure of single-layer MoS_2 is rather robust upon local deformation.

References

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[3] M. Ghorbani-Asl, R. Juarez-Mosqueda, A. Kuc, T. Heine, *J. Chem. Theory Comput.* **8**, 2888 (2012).
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