Electrical Contacts to Nanoscale Materials and Devices

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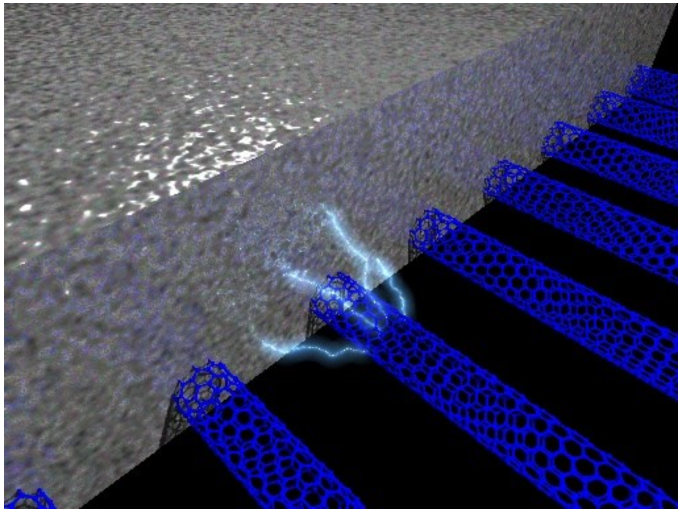
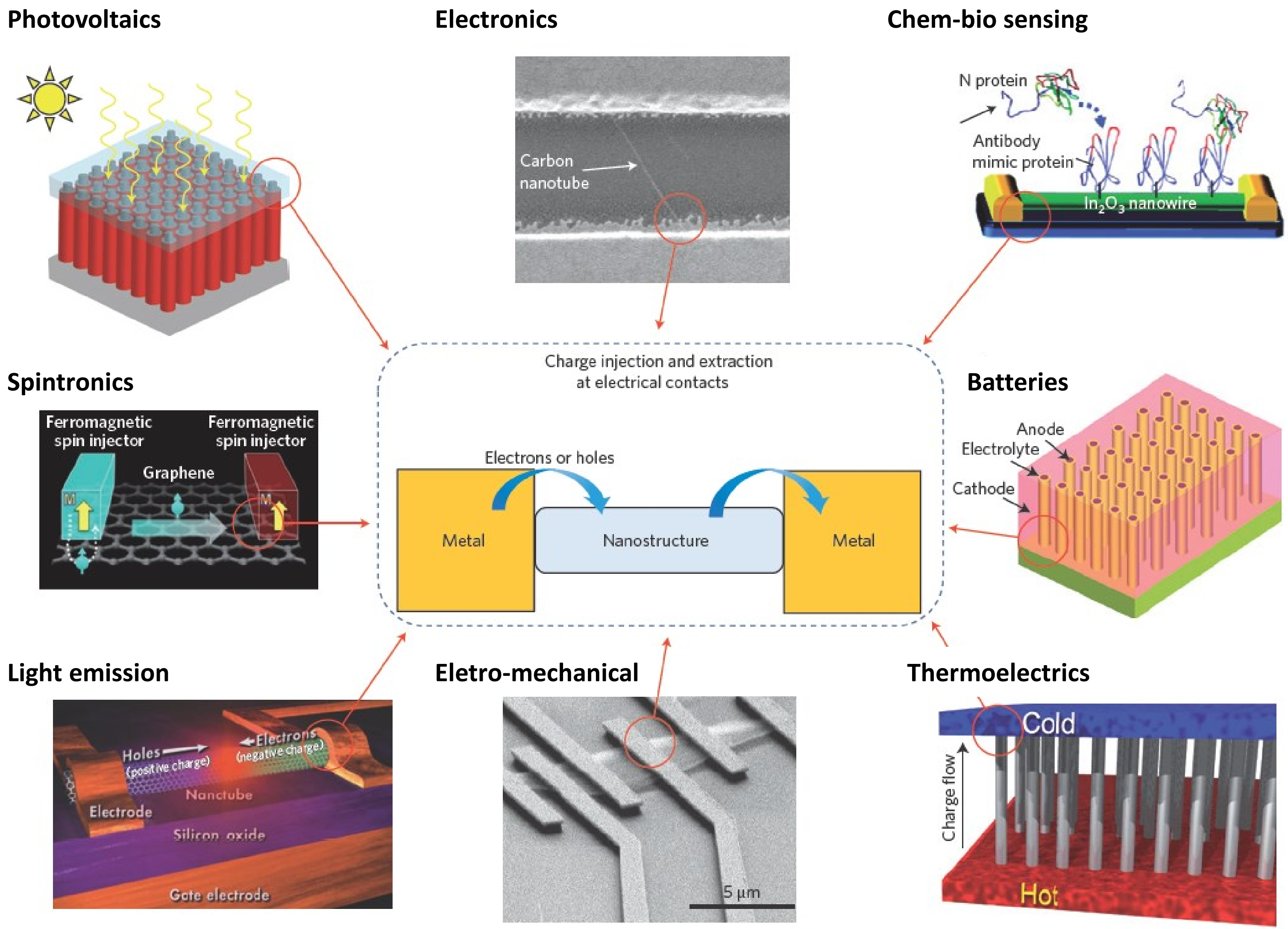
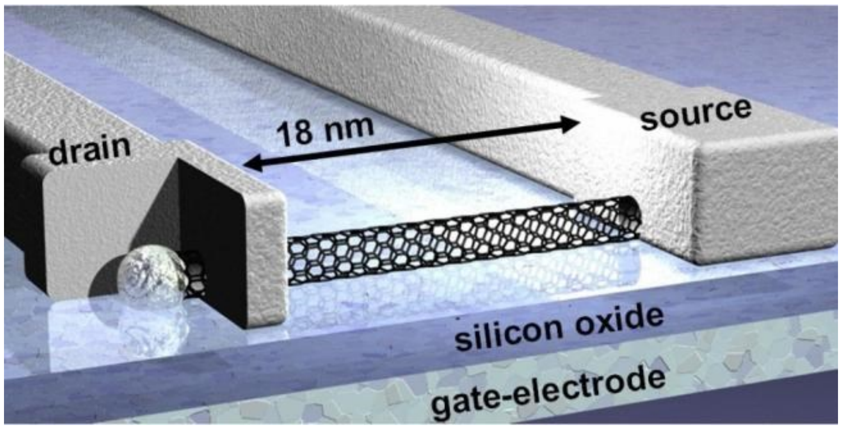


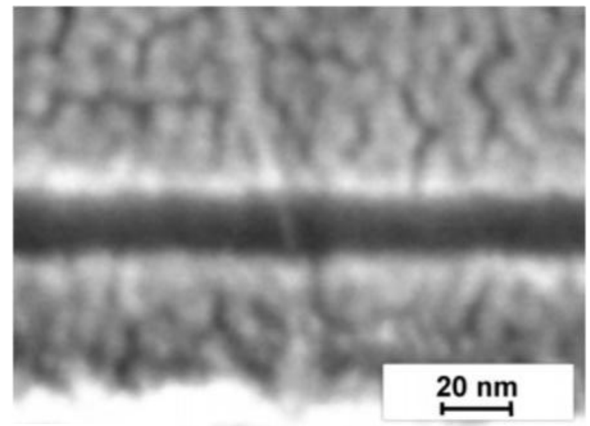
Contacts to nanomaterials are pervasive



F. Léonard and A.A. Talin, Nature Nanotechnology (2011)

Contacts are critical for nanodevices





Seidel et al, Nano Lett. (2005)

For nano-channel devices:

- **contacts are a significant physical portion of the device**
- **contact resistance can dominate over channel resistance**

Challenges and Opportunities

Characterizing nanocontacts
New contact materials
Theory and modeling
Electrical measurements
Optoelectronic measurements
Contacts to arrays
Understanding and controlling doping
Transparent contacts
High-frequency behavior
Thermal dissipation
Phase behavior
Higher–level integration
...

F. Léonard and A.A. Talin, Nature Nanotechnology (2011)

Today:

- **Ab initio modeling of contacts to topological insulators**
- **Mesoscale modeling of contacts in CNT devices**

Electrical Contacts to Topological Insulators

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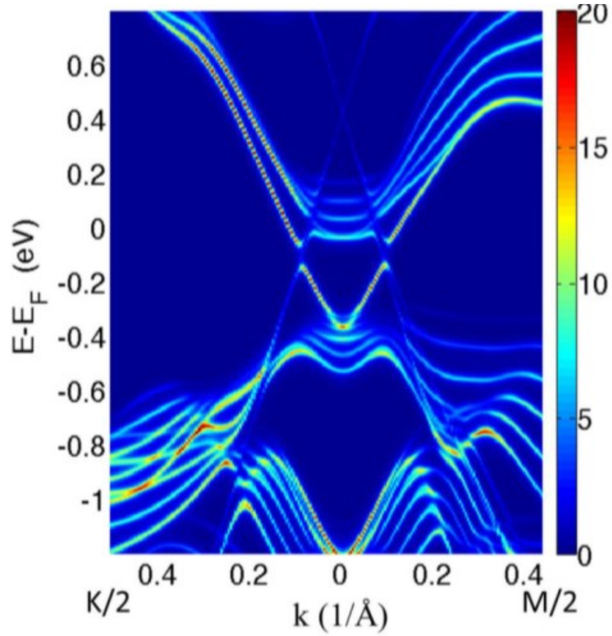
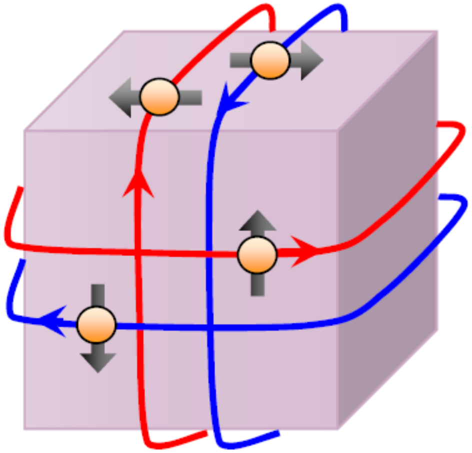
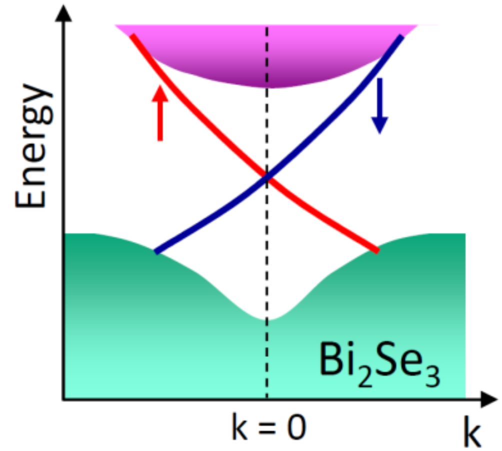
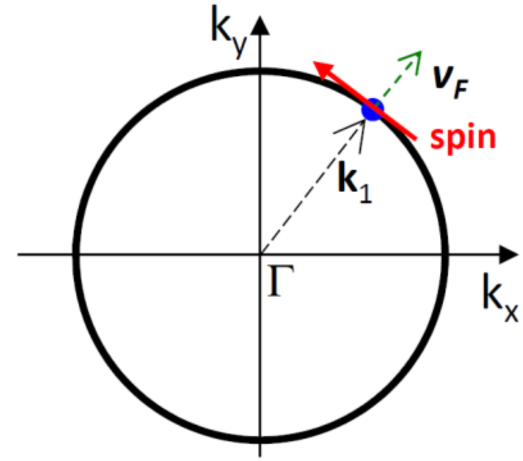


***Phys. Rev. B 90, 085155* (2014)**

Topological Insulators







Metallic surface states

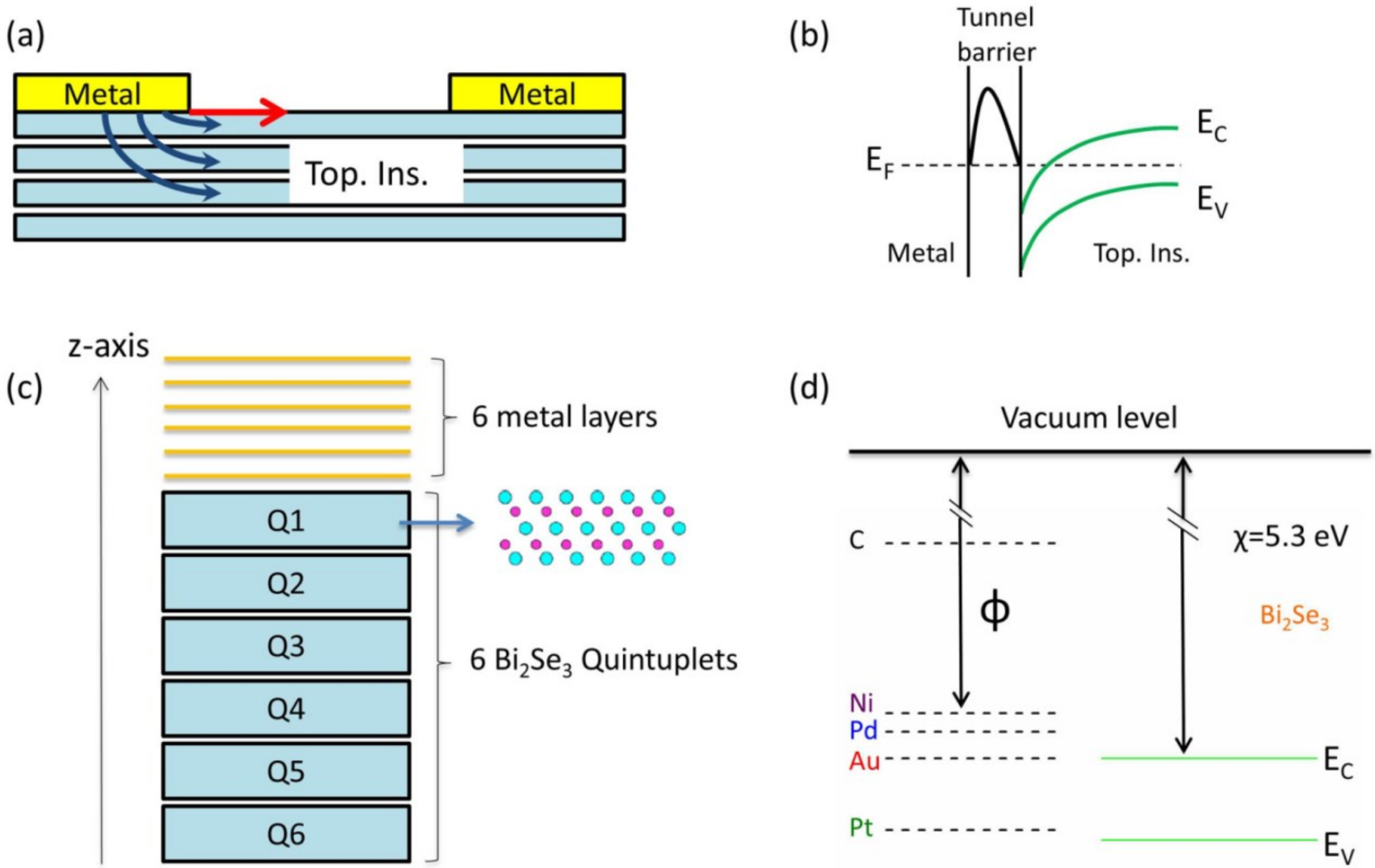
Spin-momentum locking

Need strong spin-orbit coupling

Materials: Bi_2Se_3, BiSb, Bi_2Te_3,...

Ando, J. Phys. Soc. Jpn

Important features of contacts



Approach

DFT (GGA)

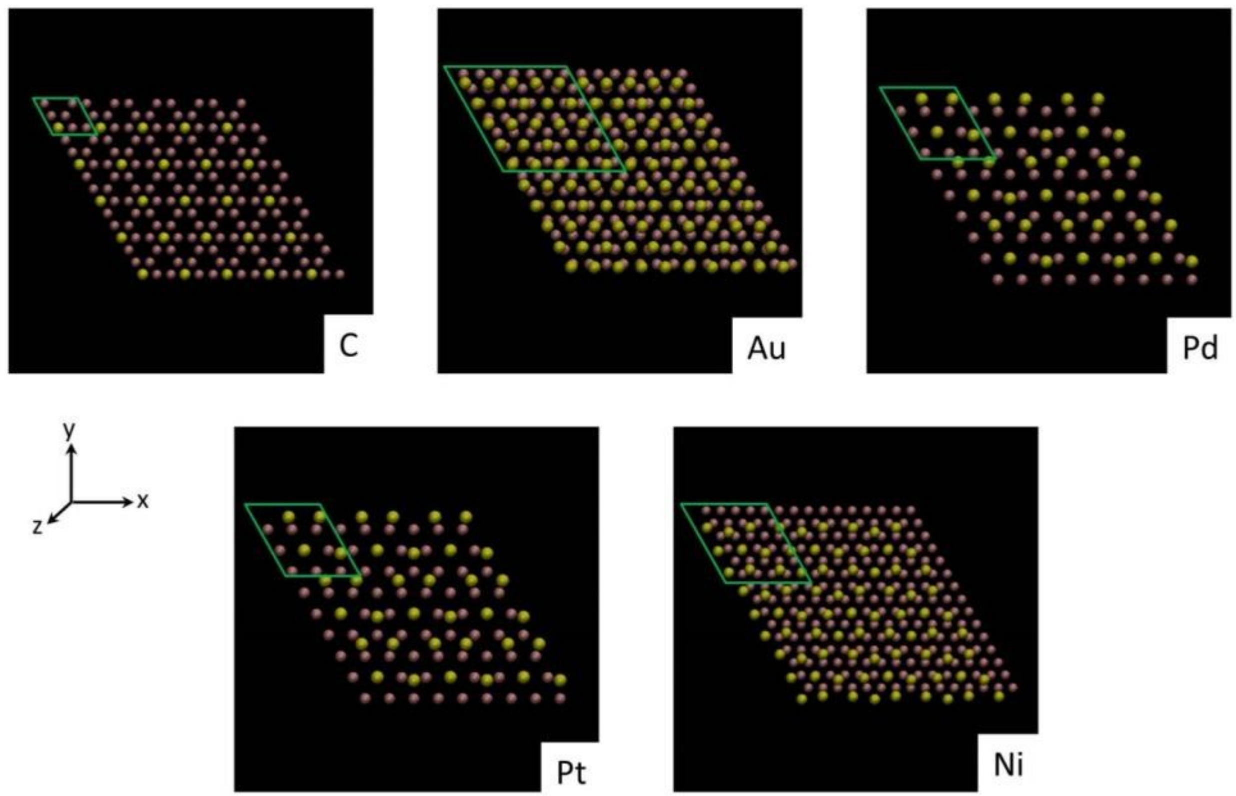
PAW pseudopotentials

Spin-orbit coupling

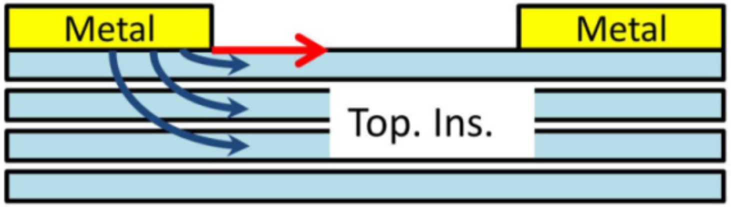
Van der Waals interactions (Grimme's method)

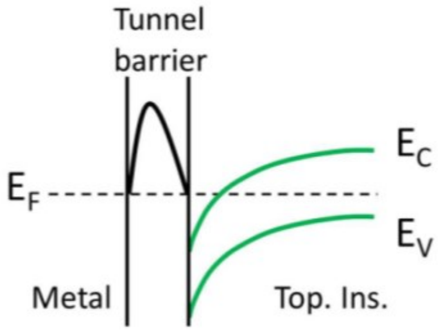
Structure relaxed

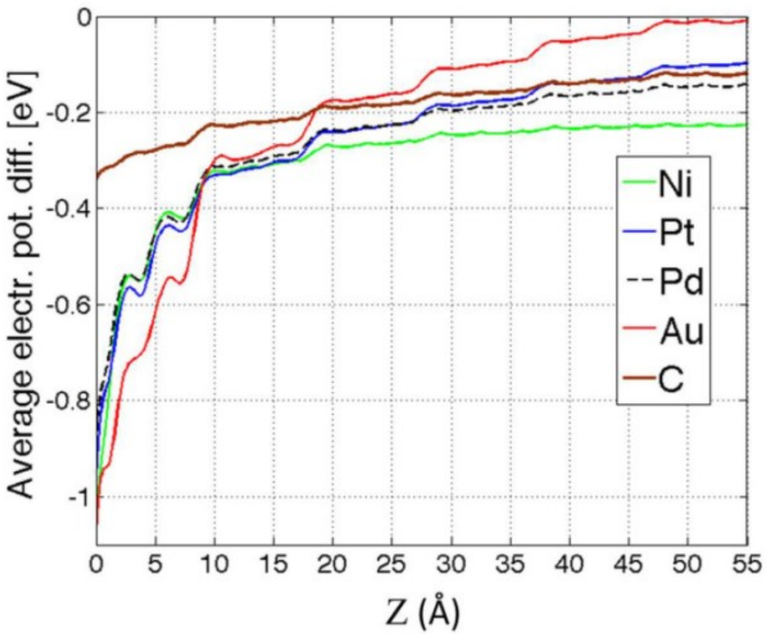
6 metal layers, 6 Bi_2Se_3 layers



Strong, n-type charge-transfer doping for ALL metals



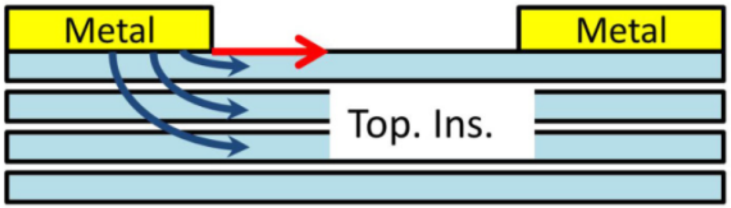


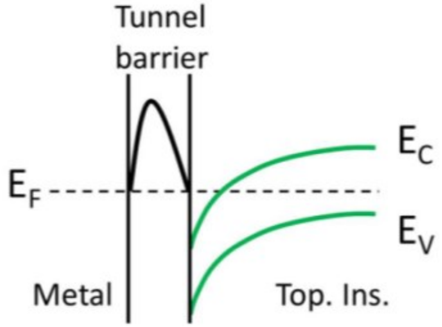


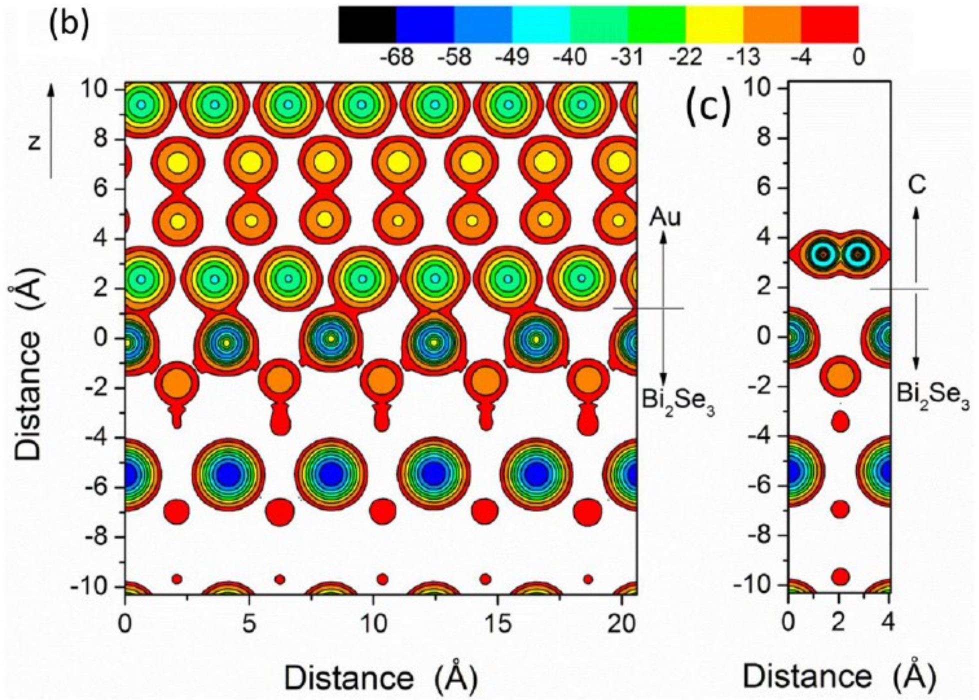
- Strong electronegativity of Bi_2Te_3 dominates over the metal workfunction
- Charge-transfer doping extends to several layers

↳ difficult to observe TI states in transport

No tunnel barriers for most metals







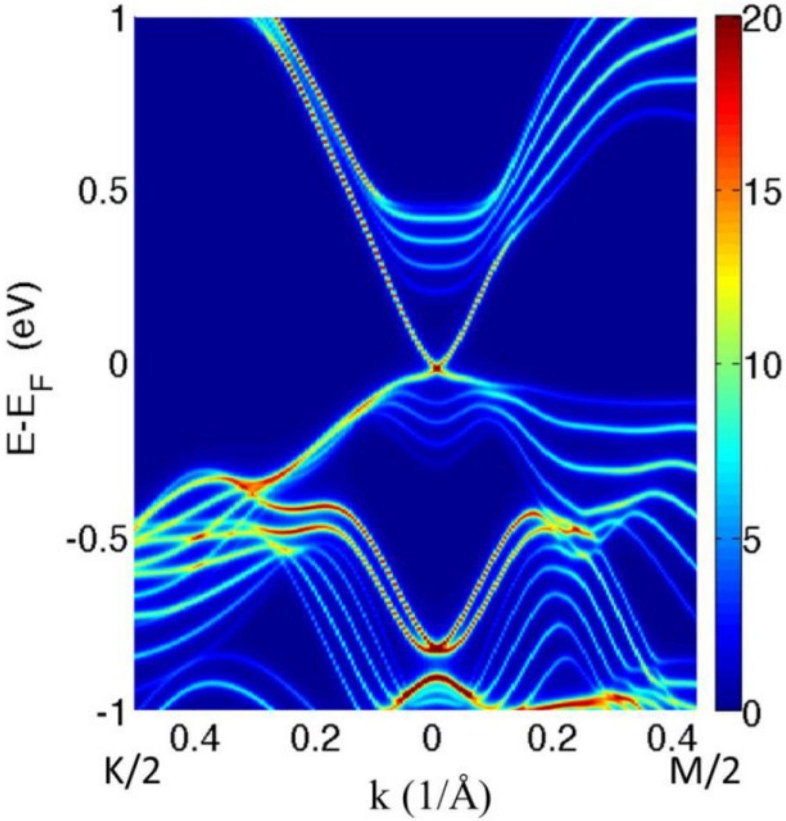
No barrier for
Au, Ni, Pd ,Pt

Graphene
has barrier

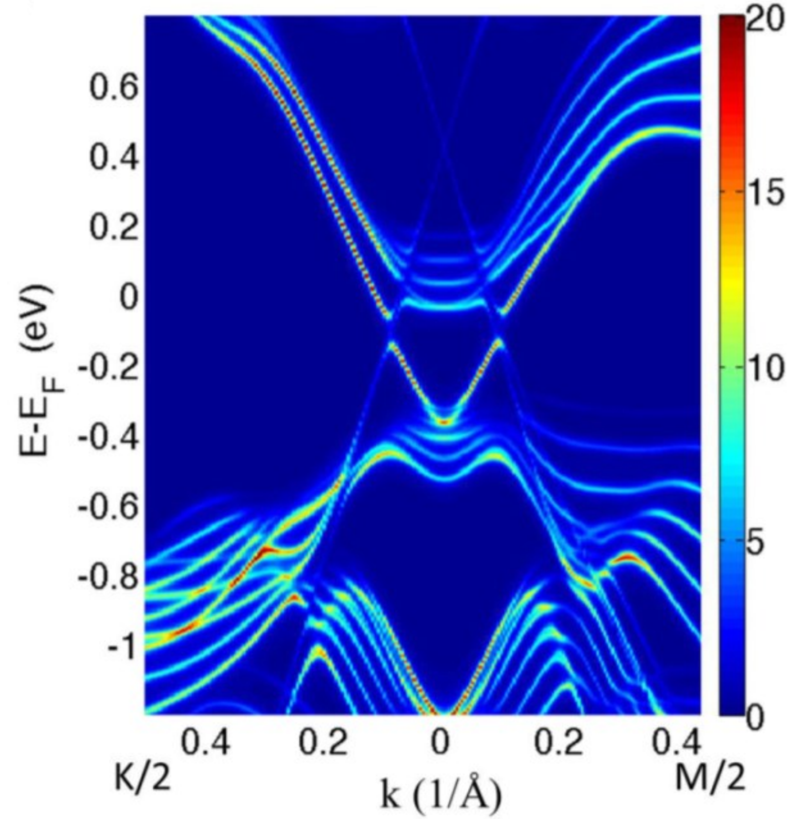
Strength of electronic interaction

$$A_j\left(\vec{k},E\right) = \sum_{n,i} w^i_{n\vec{k}} \cdots_{n\vec{k}}$$

Vacuum

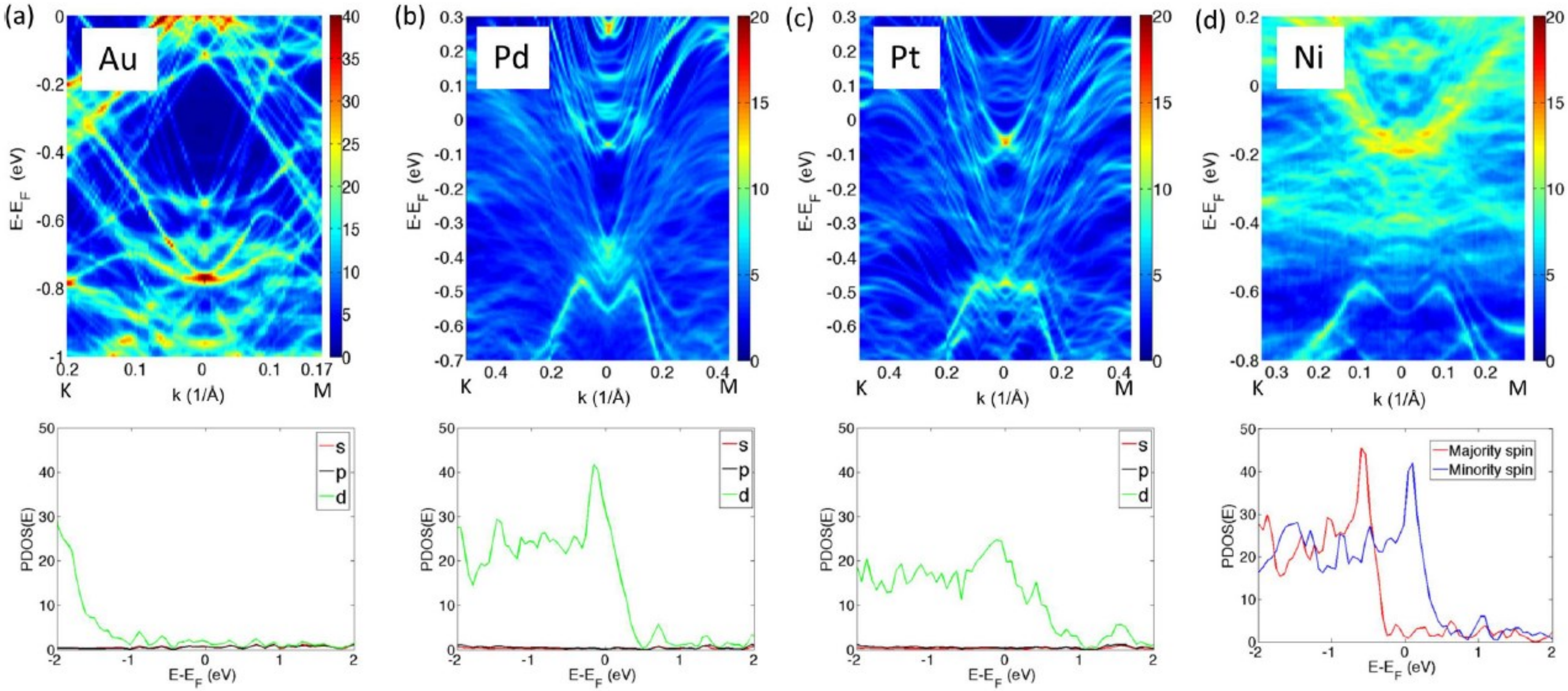


Graphene contact



- ➢ As expected, graphene binds weakly to Bi_2Se_3

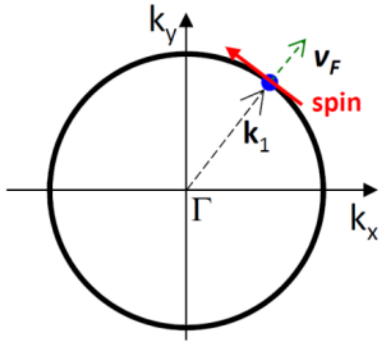
Strength of electronic interaction

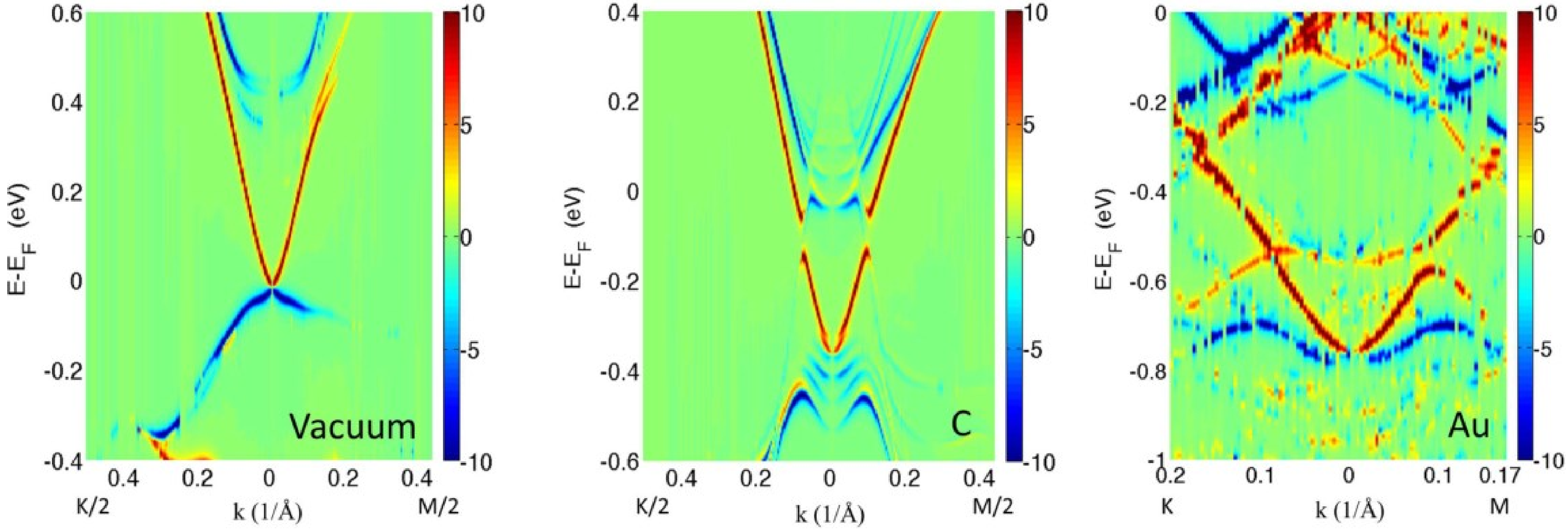


Au: weak interaction (d states well below Dirac point)
PD, Pt, Ni: strong interactions (d states near Dirac point)

Spin-momentum locking

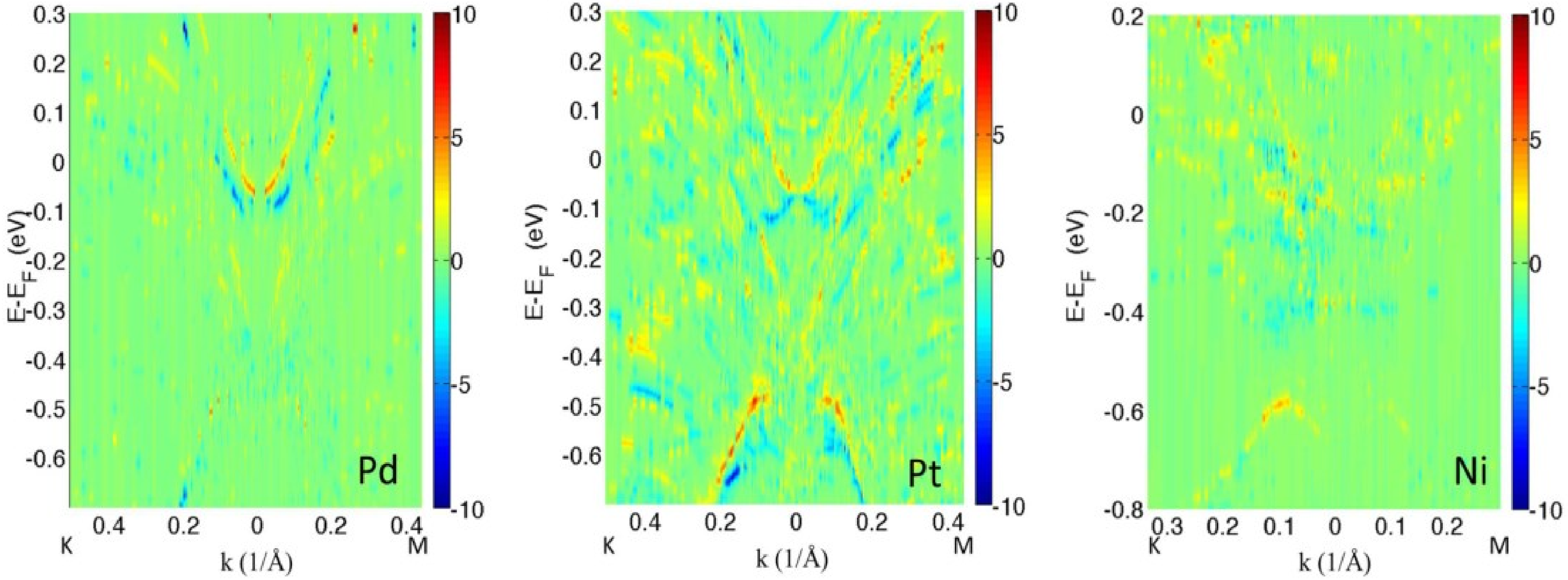
$$\hat{S}_{p_z} \cdot \left(\hat{k} \times \hat{z} \right) \approx \pm 1$$





➢ Graphene and Au maintain spin-momentum locking

Spin-momentum locking



➢ **Spin-momentum locking destroyed by interaction with metal!**

Gate Modulation of Electrical Contacts in Carbon Nanotube Devices

Aron Cummings and François Léonard

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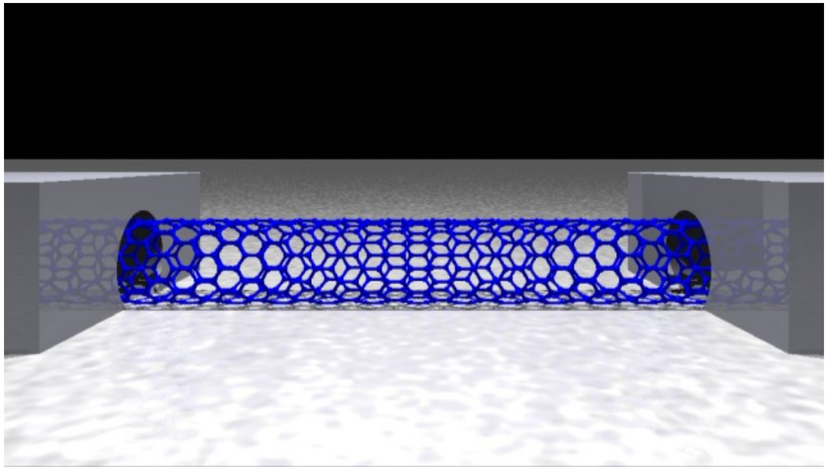
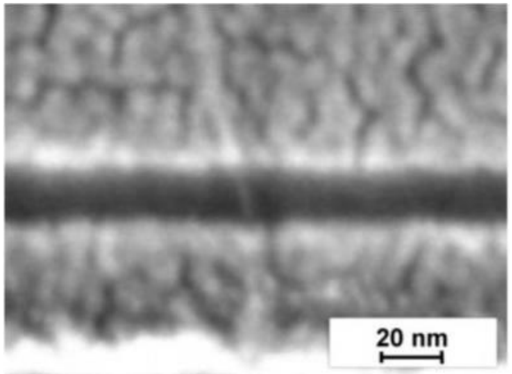
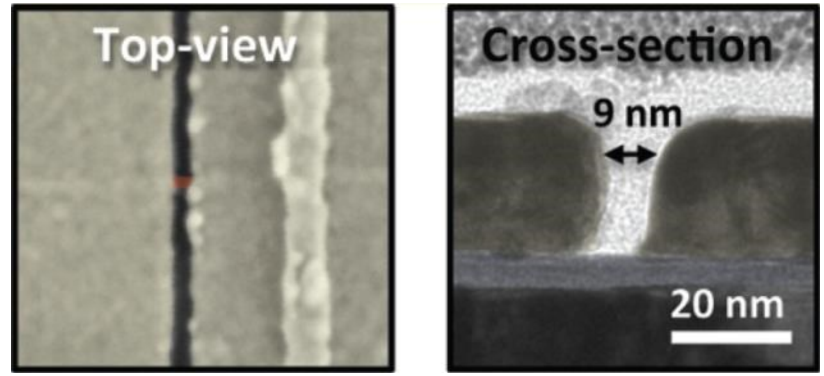


ACS Nano 6, 4494 **(2012)**

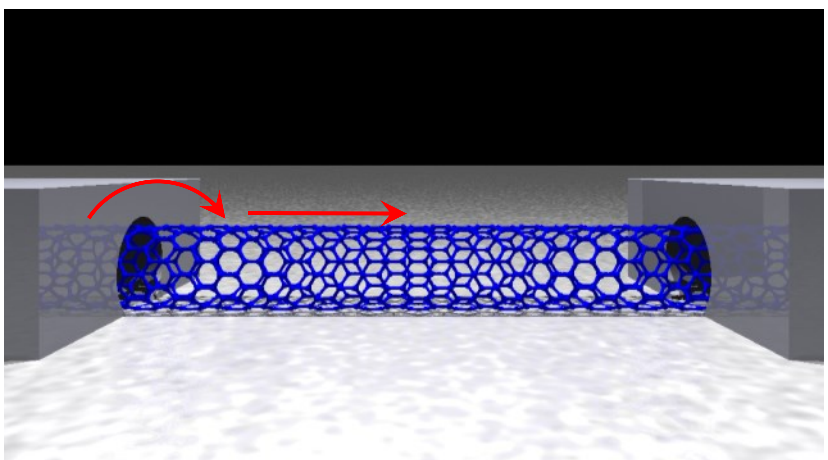
CNTFETs with ultrathin channels have now been realized:



Seidel et al, *Nano Lett*. (2005)



Franklin et al, *Nano Lett*. (2012)



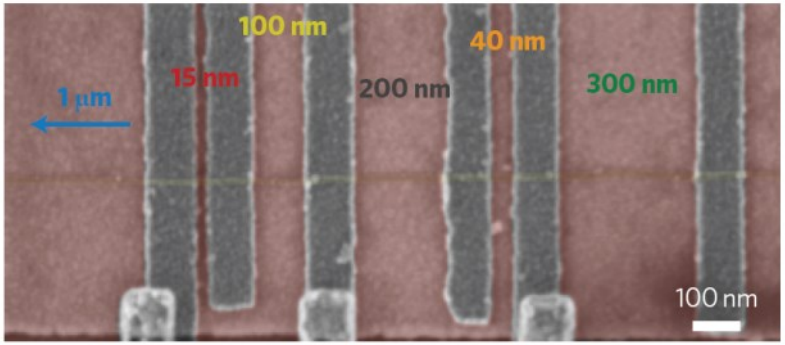
Contacts

Electronic transport

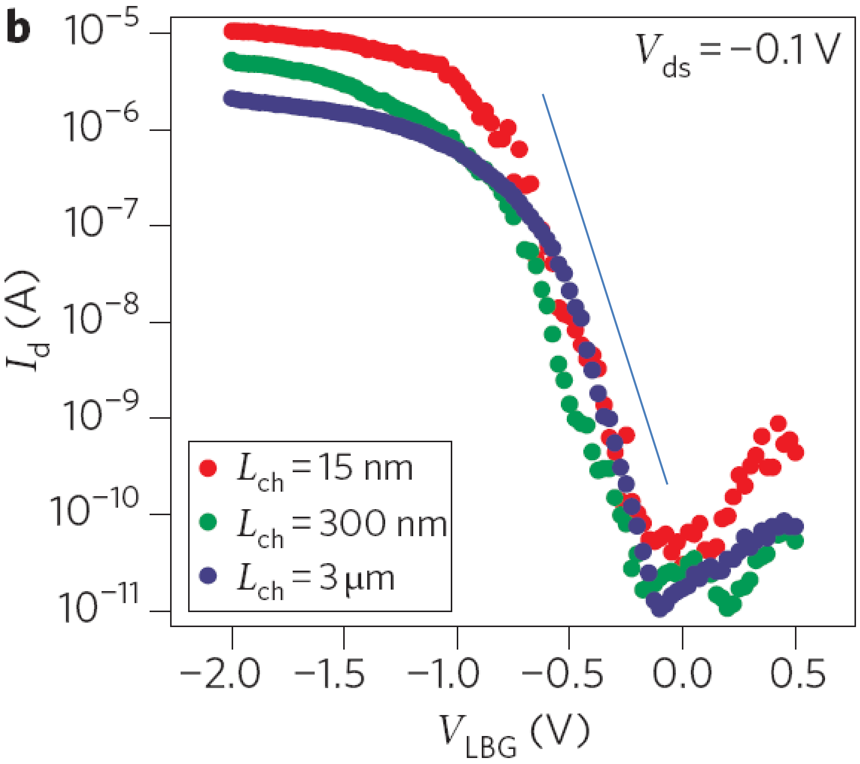
Electronic structure

Device geometry

Amazing experimental observation:

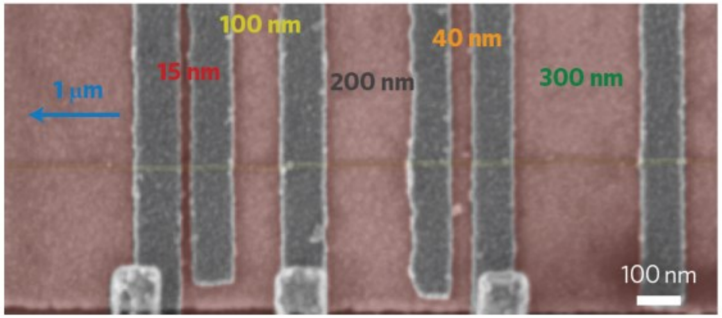


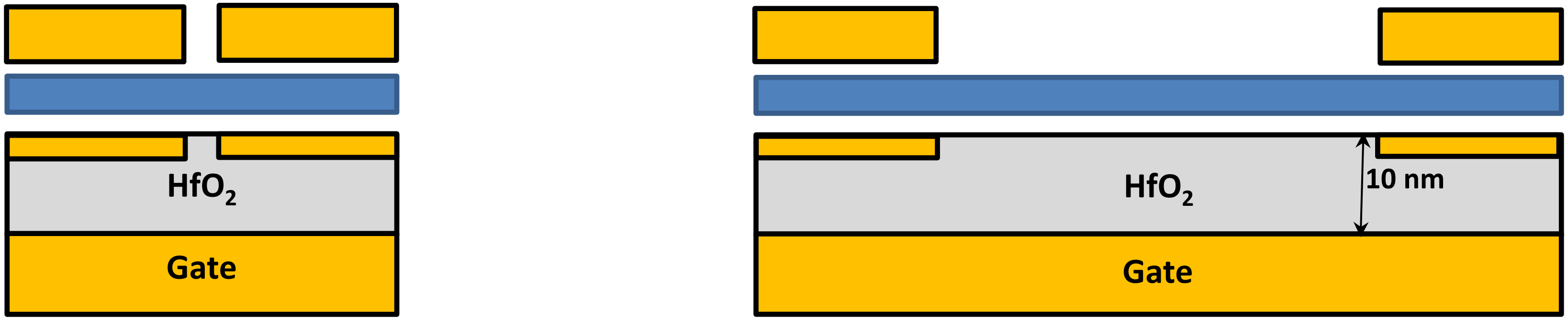
Franklin and Chen, *Nat. Nanotech.* (2011).

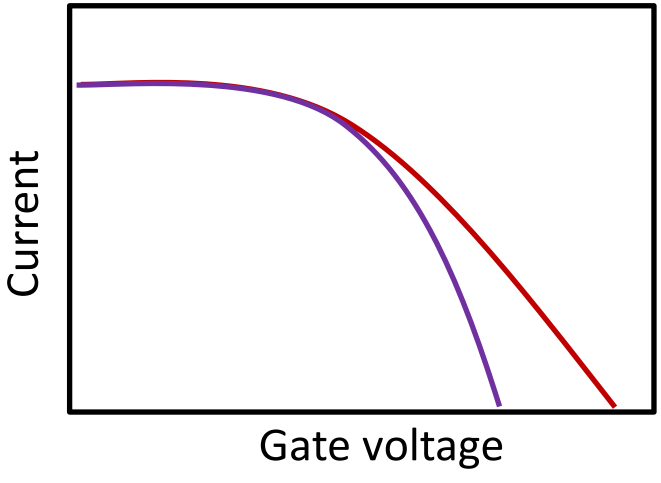


Subthreshlod swing independent of channel length !

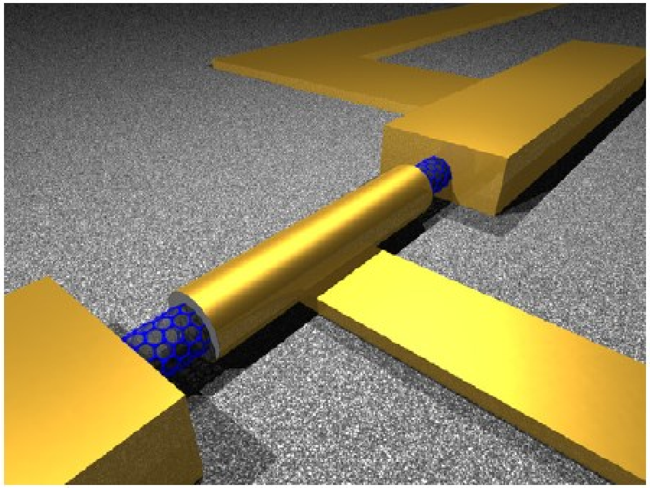
Surprising, because short-channel effects should be important at these dimensions:

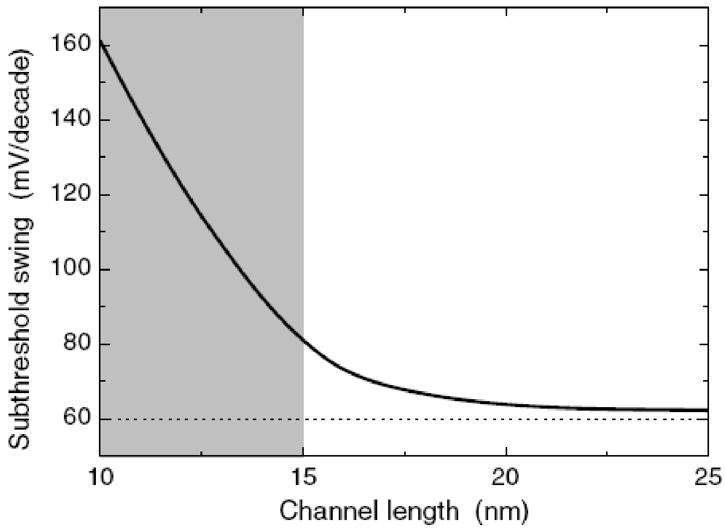






Previous modeling work has shown that a (supposedly) better design still shows strong short-channel effects:

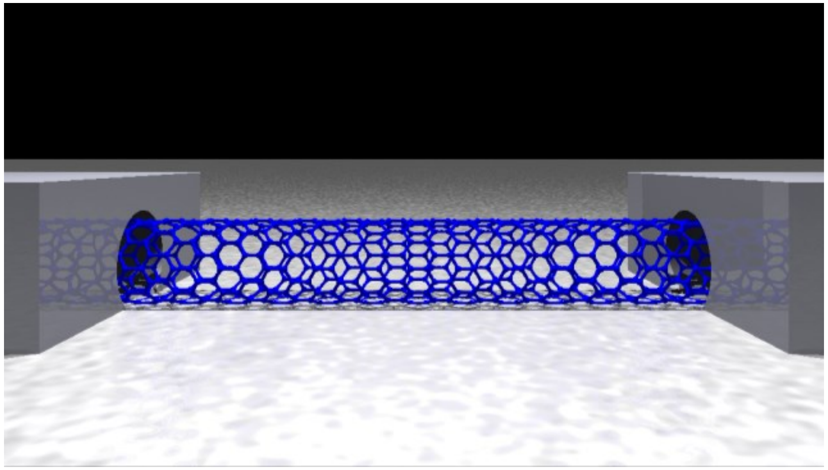




Léonard and Stewart, *Nanotechnology* (2006).

Why is experimental scaling so much better?

Modeling approach: self-consistent NEGF



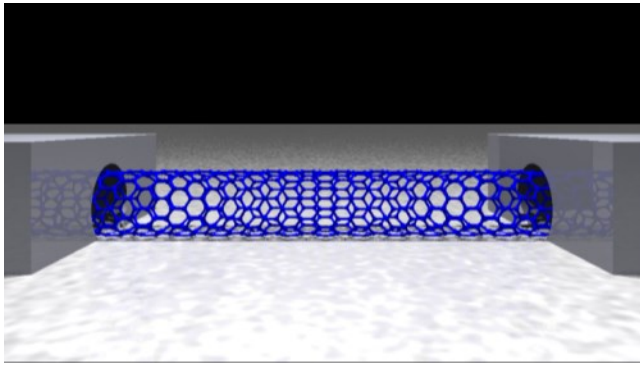
1. Solve Poisson's equation in device geometry to obtain electrostatic potential

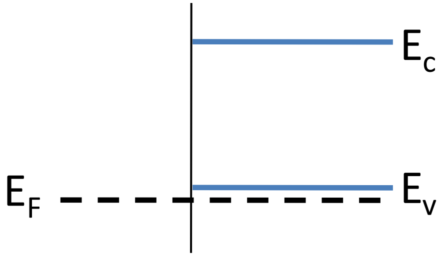
2. Use NEGF to obtain charge on CNT using tight-binding

3. Calculate current with NEGF

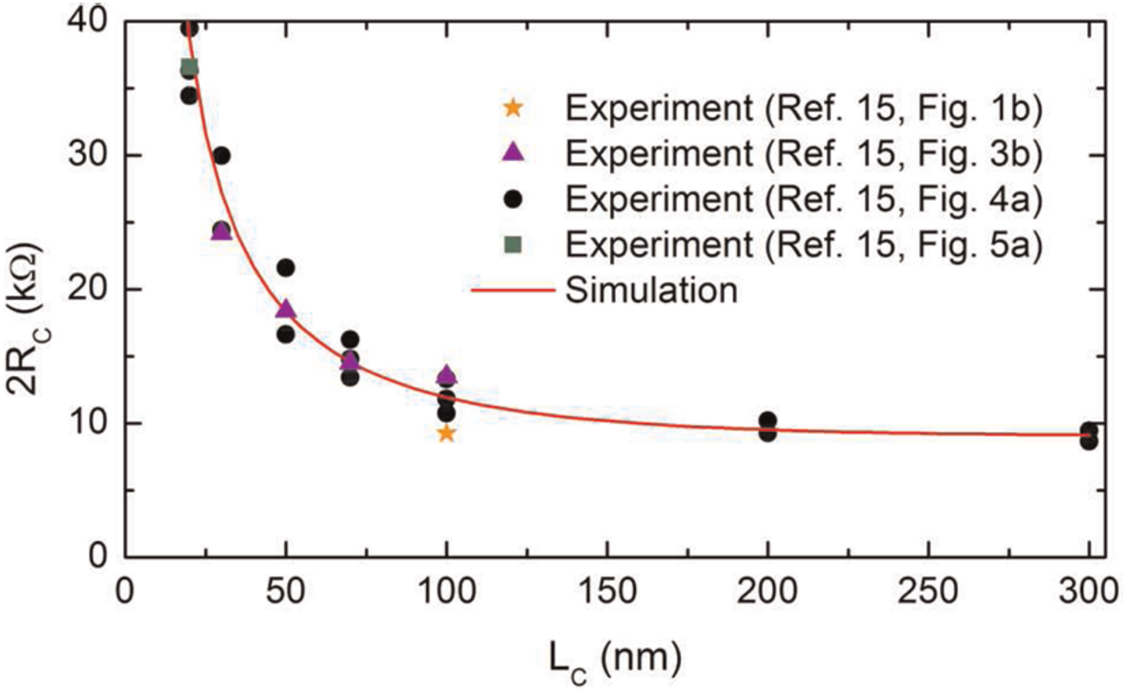
Léonard and Stewart, *Nanotechnology* (2006).
Léonard, *Nanotechnology* (2006).
Cummings and Léonard, *Appl. Phys. Lett.* (2012).

Contact parametrization



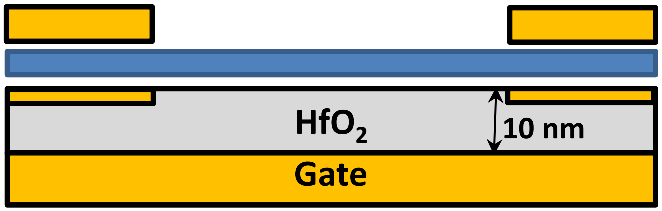


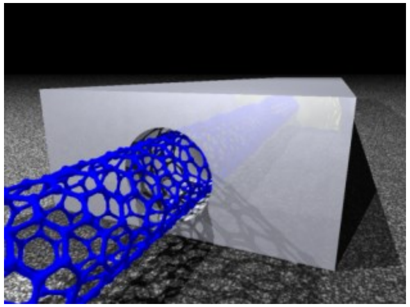
Cuniberti et al, PRL (2006).

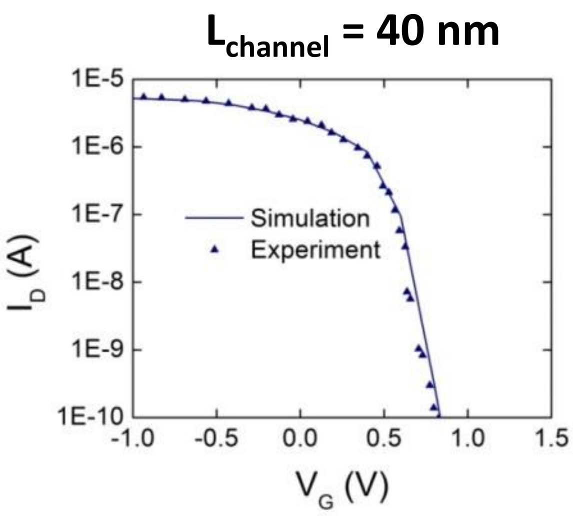


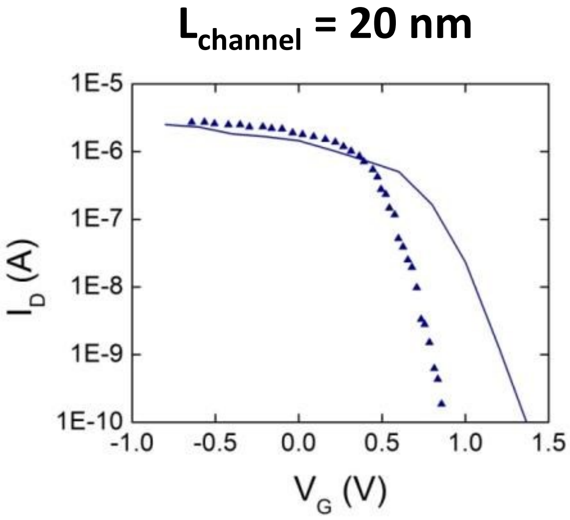
Cummings and Léonard, *ACS Nano* (2012).

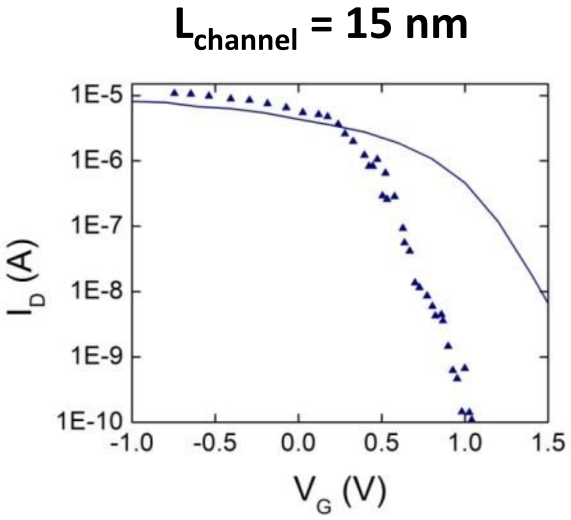
Embedded contact



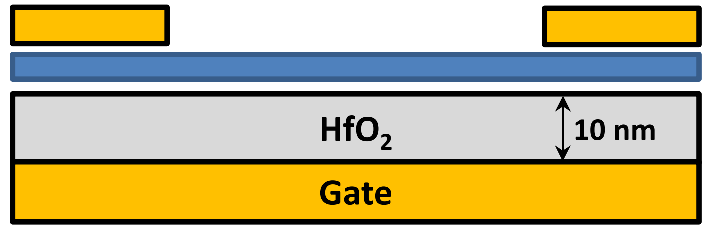


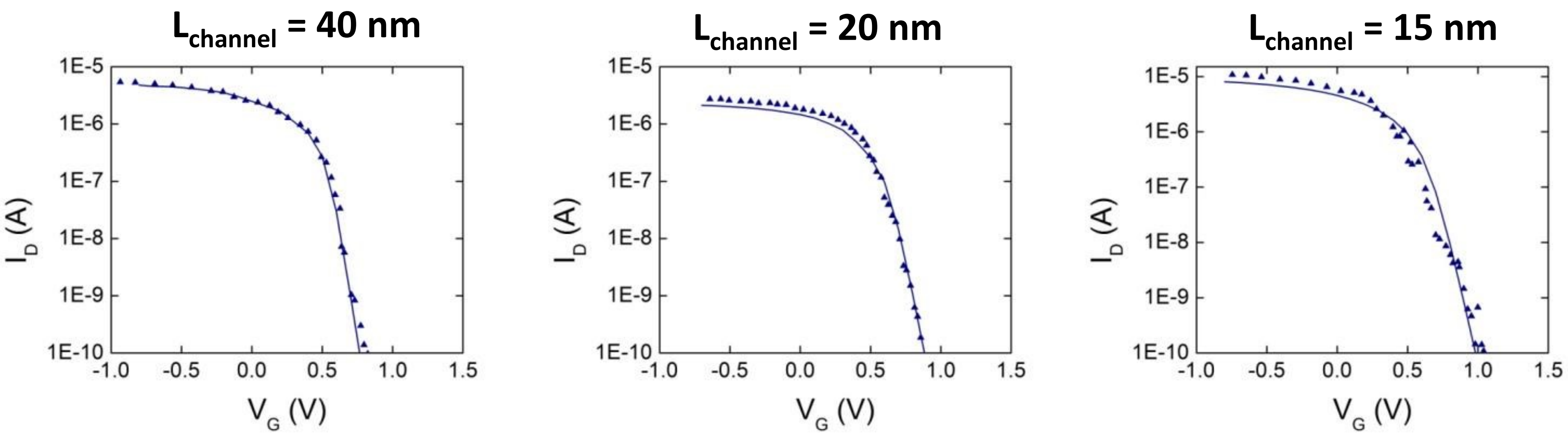






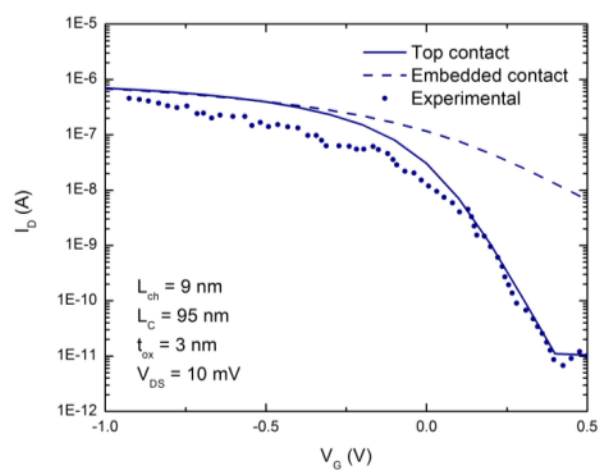
Top contact



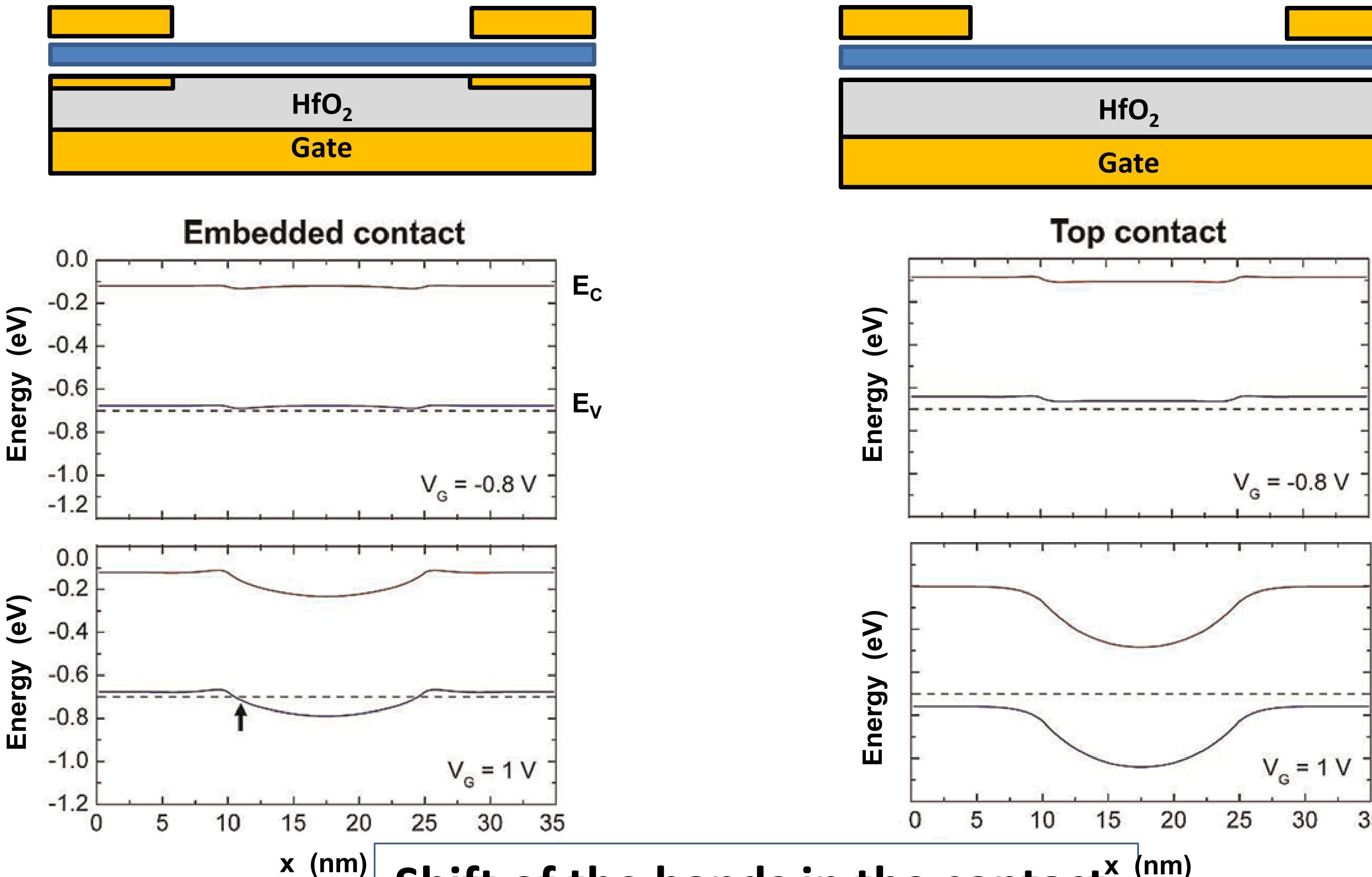


Cummings and Léonard, *ACS Nano* (2012).

Result holds for 9 nm device:



How does it work?

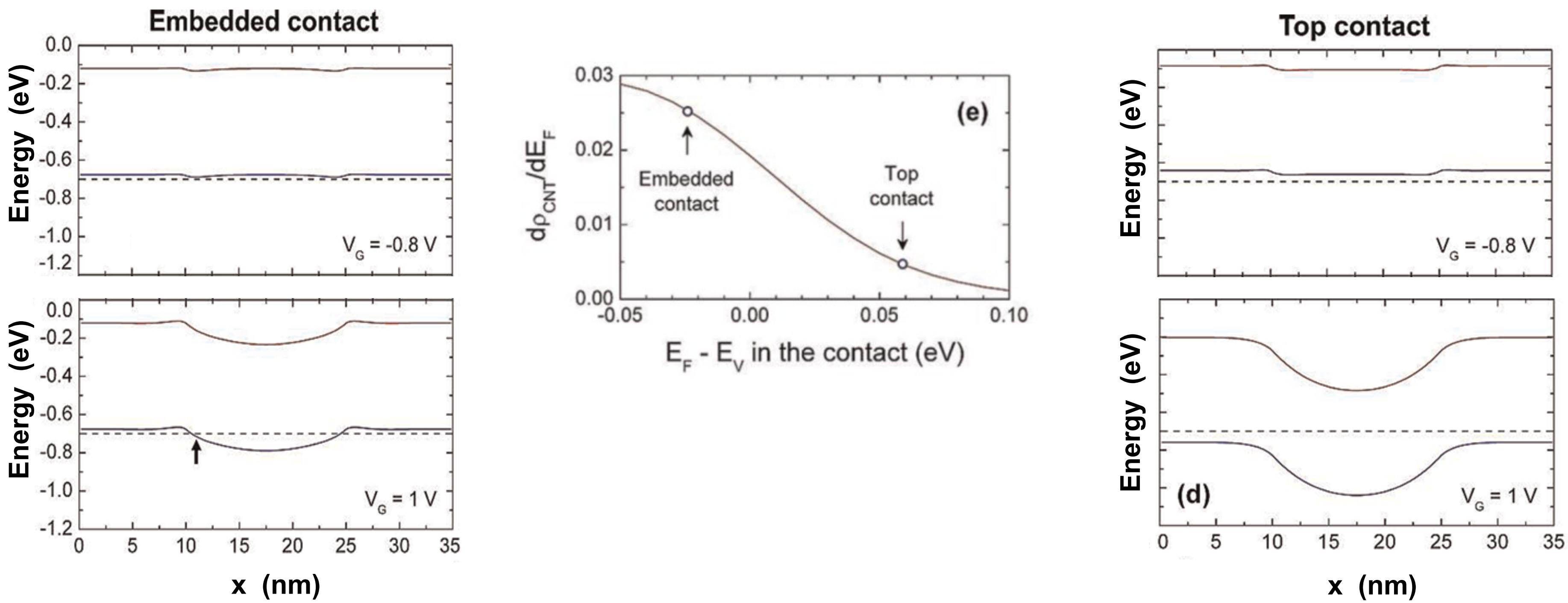


Shift of the bands in the contact

AND

Larger barrier

How does it work?

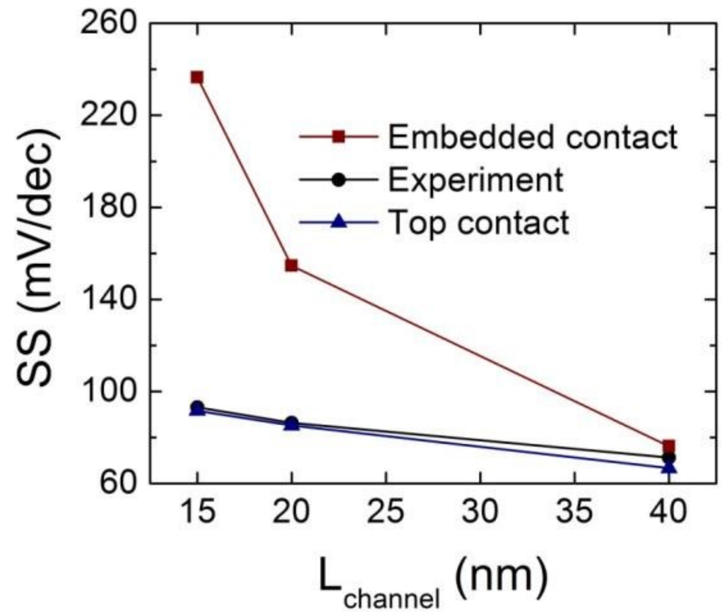


Gate modulates the contact from ohmic to Schottky

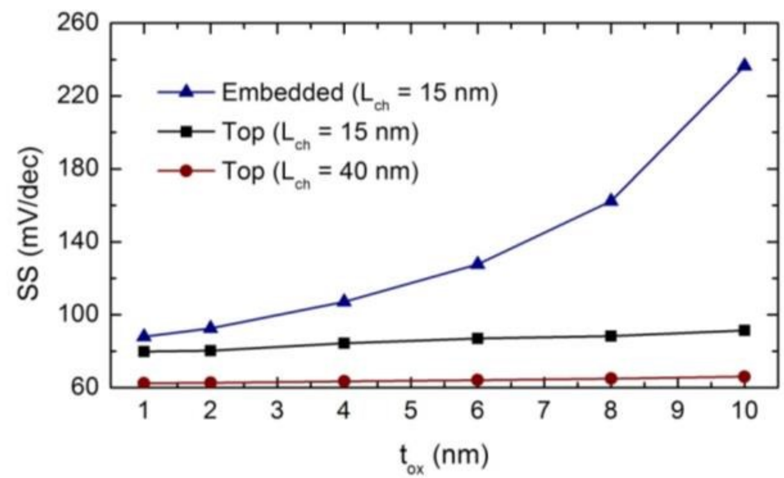
Lowers the quantum capacitance

Impact on device performance

Contact modulation gives superior channel scaling:

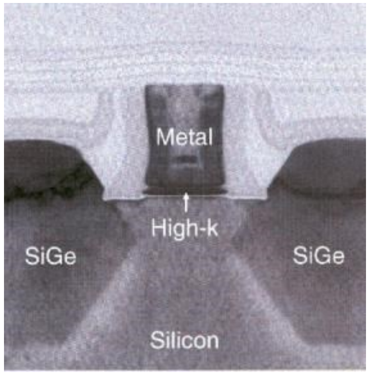


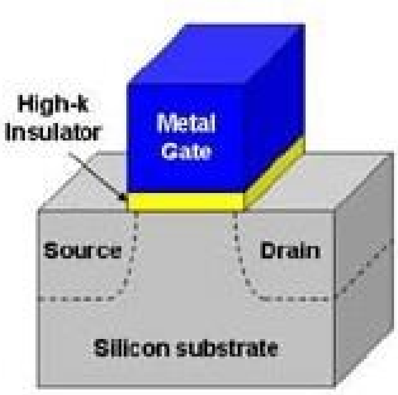
Scaling with oxide thickness also improved:



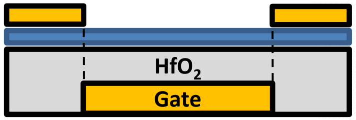
Cummings and Léonard, *ACS Nano* (2012).

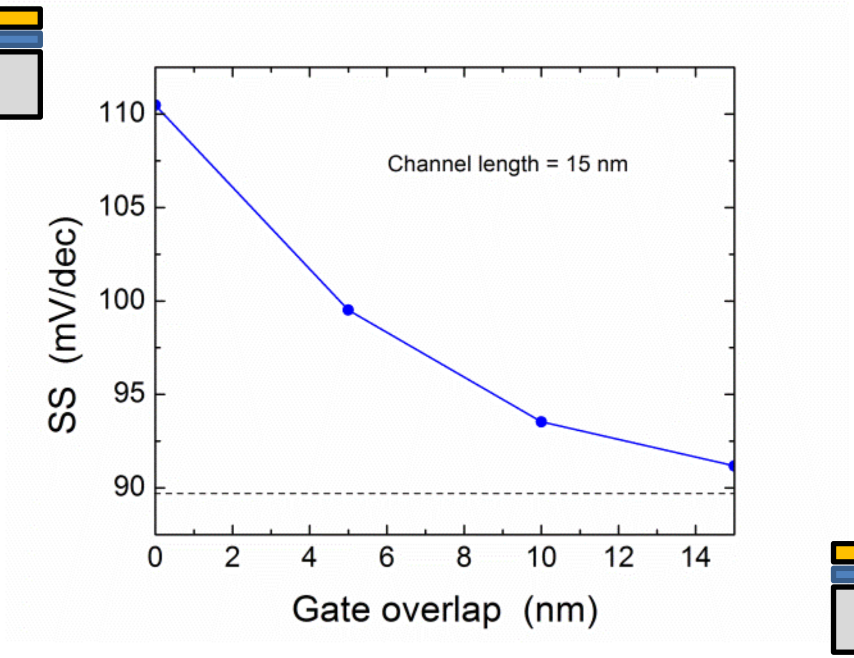
Implications for device design: gate overlap

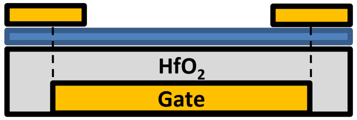




Intel





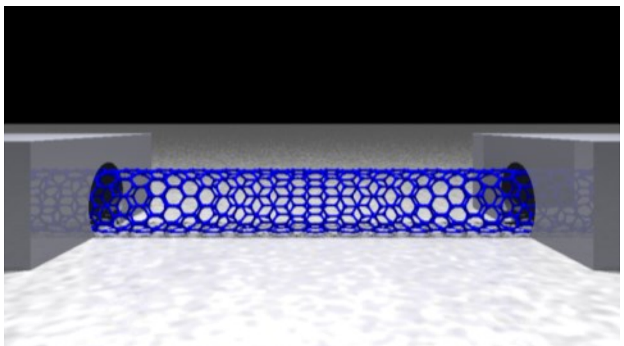


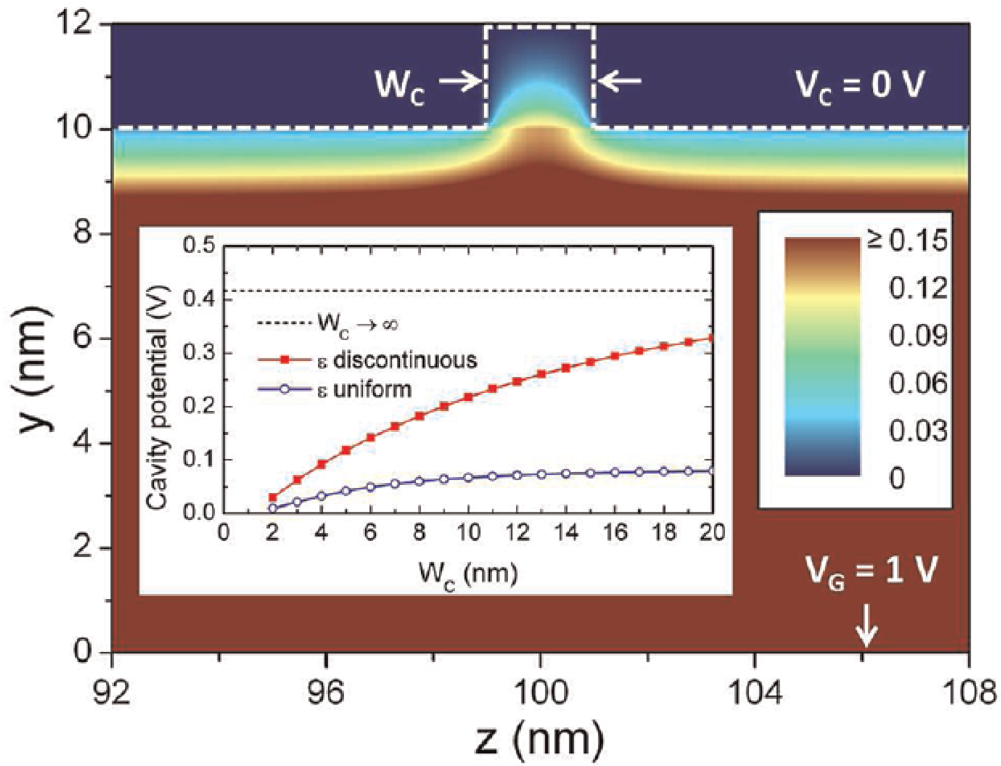
Outlook

- Device studies based on gate modulation of contacts
- Non-equilibrium transport (e.g. current saturation)
- Including many-body effects in device simulations
- Contacts (structure, electronic properties, transport)

This work is supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Fields are able to penetrate cavity because of field enhancement due to discontinuity in dielectric constants





Quantum vs classical capacitance

$$\frac{C_{cl}}{length} = \frac{2\pi\varepsilon}{\ln(4h/d)} \;\square \qquad\qquad \text{m}$$

$$\frac{C_Q}{length} = e^2 D(E_F) \;\square \qquad\qquad \text{m for metallic CNT}$$

Subthreshold swing for FinFET