Field Regulation of Single Molecule Conductivity by a Charged Atom

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Cartoons useful but can mislead


Break junctions
- McEuen for example
- break, pour, electrical change,
- assume got molecule
- no knowledge of electrode structure, of position, configuration, number of molecules
- gate inefficiency, ~1%, so need ~100V to get 1V at molecule
- this limits what can be done (breakdown occurs ~< 30 V, so do Kondo)
- need cryogenic
Our Approach is Different

• Use STM, see where the atoms are
• Because details known, can do detailed modeling
• Visualize electric field
• We make 2 electrodes that, in a limited way, act like 3
• Study true field effect

Our Results

• Show chem and spatial gating, show what gating will act like when an eventual third electrode is obtained

• Ideal Gating Efficiency => Room temperature
• 1 not 100,000 electrons to gate => low power, high speed
• built upon silicon => merge old and new
• small size => potential for speed
Field regulation of single-molecule conductivity by a charged surface atom
Paul G. Piva, Gino A. DiLabio, Jason L. Pitters, Janik Zikovsky, Moh’d Rezeq, Stanislav Dogel, Werner A. Hofer & Robert A. Wolkow
3 points to discuss

1. Fabrication of Dangling Bond/Molecule/Si

2. Nature of dangling bond

3. Field effect shifts molecular energy levels
The juxtaposition of Molecule(s), Dangling Bond and Silicon surface can be done automatically

\[ \text{~18 years of preparation allows us to know structure} \]


Poisson Calcs
Janik Zikovsky

\[ \nabla^2 \phi = -\frac{\rho}{\varepsilon} \]

\[ \rho(x) = N_D \frac{2}{\sqrt{\pi}} F_{1/2} \left( \frac{E_F - E_D}{kT} \right) - N_C \frac{2}{\sqrt{\pi}} F_{1/2} \left( \frac{E_C - E_F}{kT} \right) + \frac{N_D}{1 + 2e^{\frac{E_D - E_F}{kT}}} \]

\[ \sigma = \sigma_{DB} \left( 1 - \frac{1}{1 + \exp\left( \frac{E_D - E_F}{kT} \right)} \right) - \frac{1}{1 + \exp\left( \frac{E_A - E_F}{kT} \right)} \]

\[ \sigma = \sigma_{DB} \left( \frac{1}{1 + \exp\left( -\frac{E_D - E_F}{kT} \right)} - \frac{1}{1 + \exp\left( \frac{E_A - E_F}{kT} \right)} \right) \]

\[ \sigma = \sigma_{DB} \left( \left[ 1 + e^{\frac{E_F - E_D}{kT}} \right]^{-1} - \left[ 1 + e^{\frac{E_A - E_D}{kT}} \right]^{-1} \right) \]

Figure 2: FEM triangular meshing in the tip region.


Stark effect, see for example Herzberg, G. Atomic Spectra and Atomic Structure 2nd edn, Ch. II, 114 (Dover, New York, 1944)
Pause to comment on NDR
• There is no NDR effect for styrene on silicon
• There is a bond breaking phenomenon that masquerades as NDR
• In this talk styrene bonded differently to silicon
  – But still, no NDR
  – In this case no NDR-like spectra (because stronger bonding)
Alignment of energy levels

Charged DB shifts molecular levels up Causing molecules to “light up” at low voltage

Silicon  Styrene  Gap  Tip

CB ~4.0 V

E_{F,\text{Silicon}}

VB ~5.1 V

Styrene

E_{\text{LUMO}} \sim 1\text{V}

Styrene

E_{\text{HOMO}}

E_{F,\text{Tip}} (~ 4.5 \text{ eV no ext. bias})
Dangling bond capping $\Rightarrow$ Charge elimination and therefore Field elimination
Also single molecule sensing

High Doped

Electrons move to surface, bands bend

Low Doped

Neutral Dangling Bond
Figure 2 | Absence of charge field effects on low-doped silicon. The image shows that styrene lines on low-doped n-type H–Si(100) have no slopes. The dangling bonds (indicated by arrows) are neutral under the imaging conditions used (sample bias $-2.0$ V and $80$ pA), and no significant height perturbation is observed along the molecular lines. Image area is $15$ nm $\times$ $15$ nm.
Conclusions

- Because we use STM
  - See where the atoms are (know if molecule present, where and in what configuration)
  - Visualize electric field
  - Structure known, can do detailed modeling
    - Modeling -> structure property relationship -> for example tuned onset voltage

- Because we understand 1) surface chem, and 2) band effects, and 3) field effects
  - Can create a single charged atom next to a molecule
  - Can make 2 electrodes that, in a limited way, act like 3

- Show chem and spatial gating, shown what gating will act like when an eventual third electrode is obtained

- Ideal Gating Efficiency  =>  Room temperature
  - 1 not 100,000 electrons to gate  =>  low power, high speed
  - built upon silicon  =>  merge old and new
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