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WEIZMANN INSTITUTE OF SCIENCE

New organic treatment for n-Si
En route to
Si Inversion layer Solar Cell

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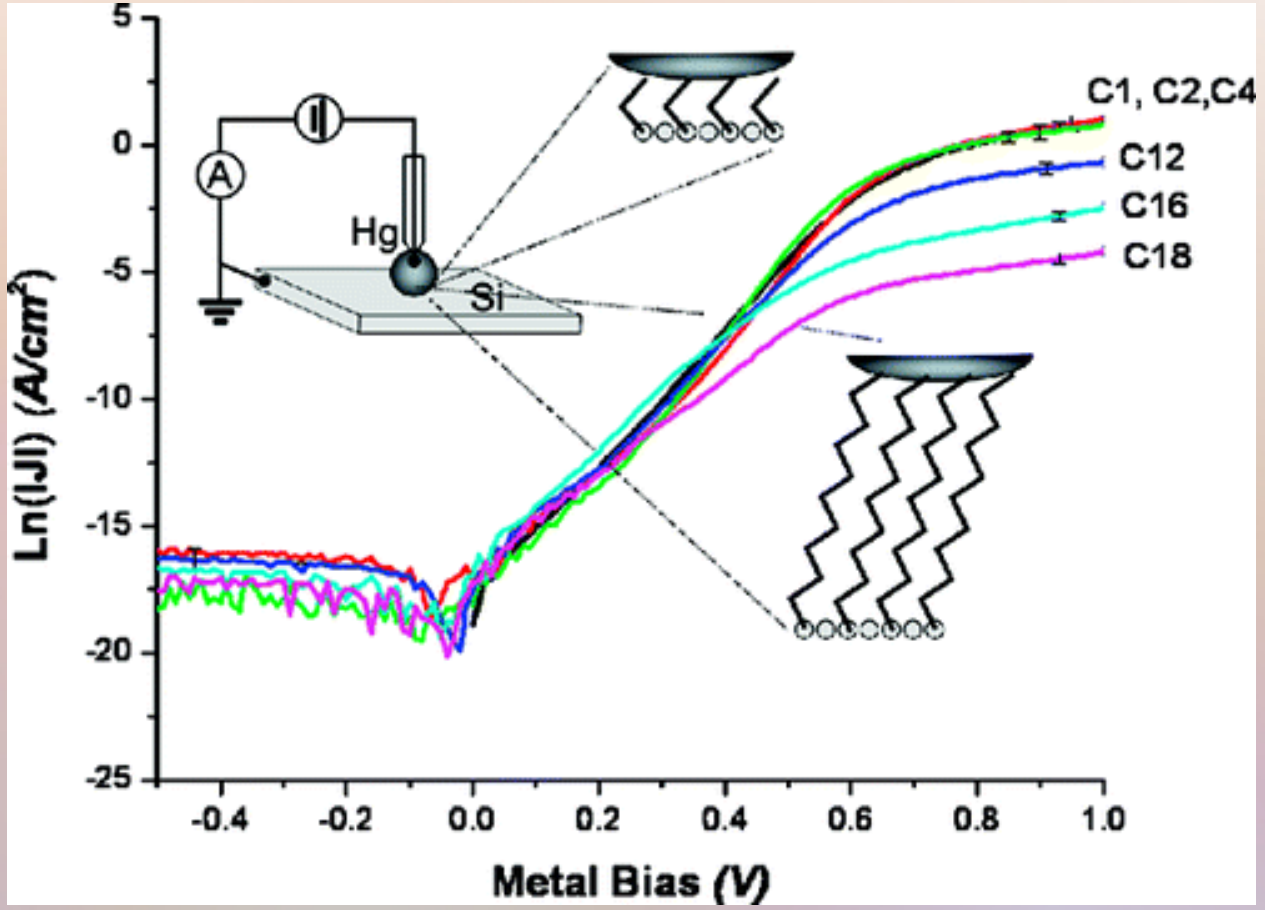
OUTLINE

- Si inversion with molecules – how it all began
  - Length independence transport of SAM on Si
  - Short reminder – Schottky barrier
  - Role of the molecules
  - What is it good for?
- Even milder conditions
- Hg drop top electrode - preliminary results
  - Varying the Si doping
- Summary

Self-assembled alkyl monolayers on n-Si

For negative and low forward bias regimes current is independent of molecular thickness.

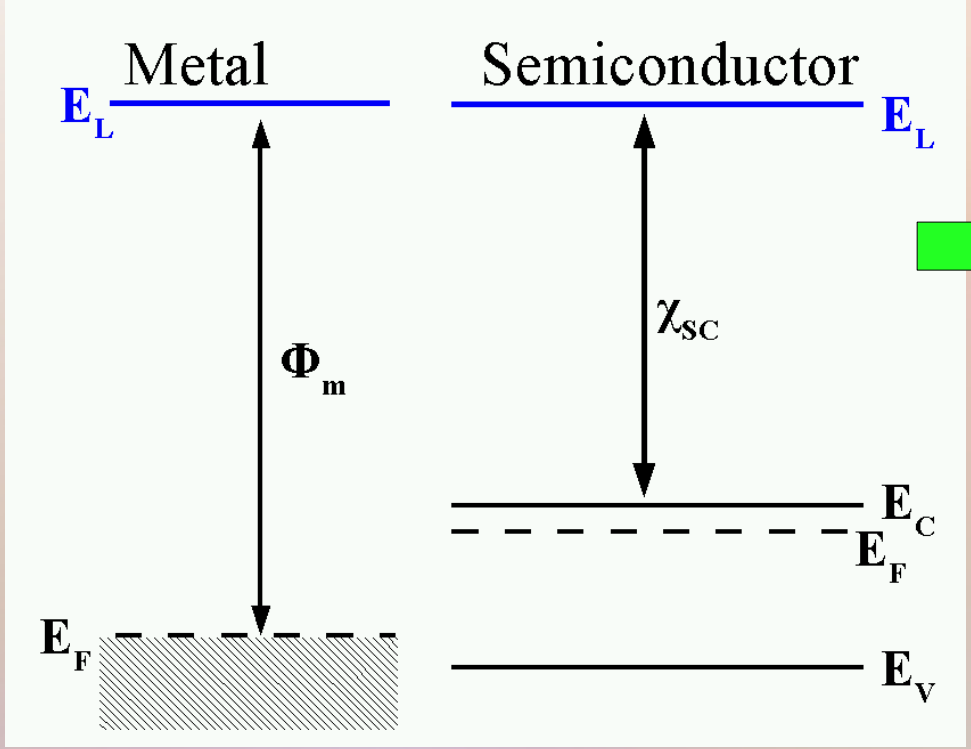


The transport bottleneck (rate limiting step) for those junctions is the semiconductor, rather than the molecules.

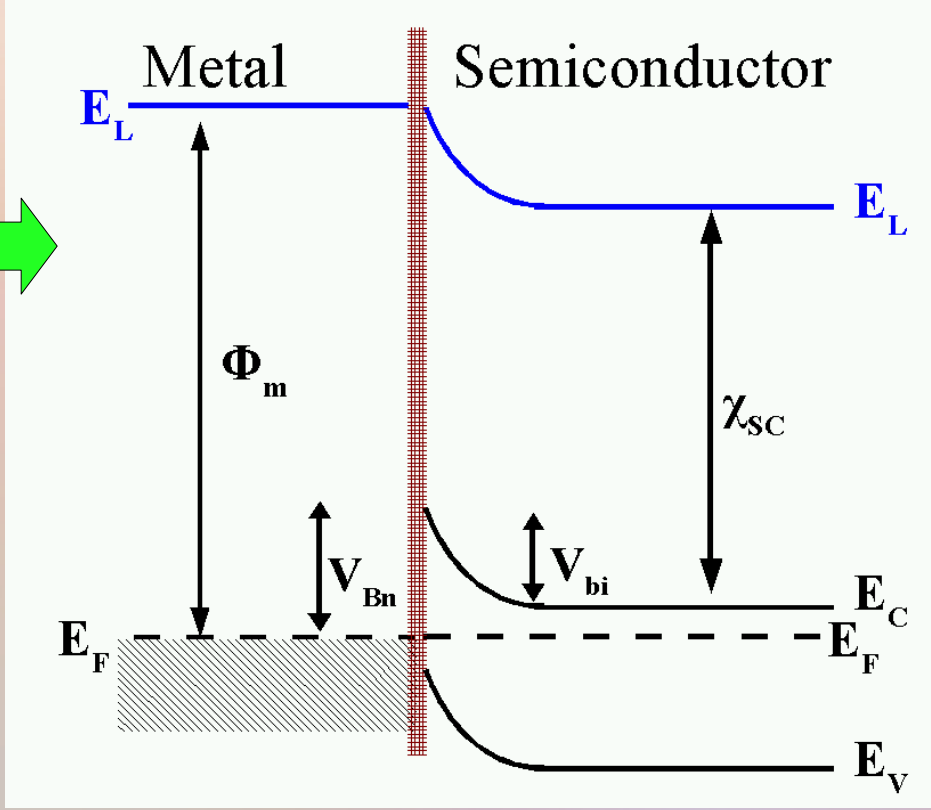
Yaffe O. et al, *NanoLetters, 9(6), 2009*

Schottky-Mott ideal picture

a) Before contact



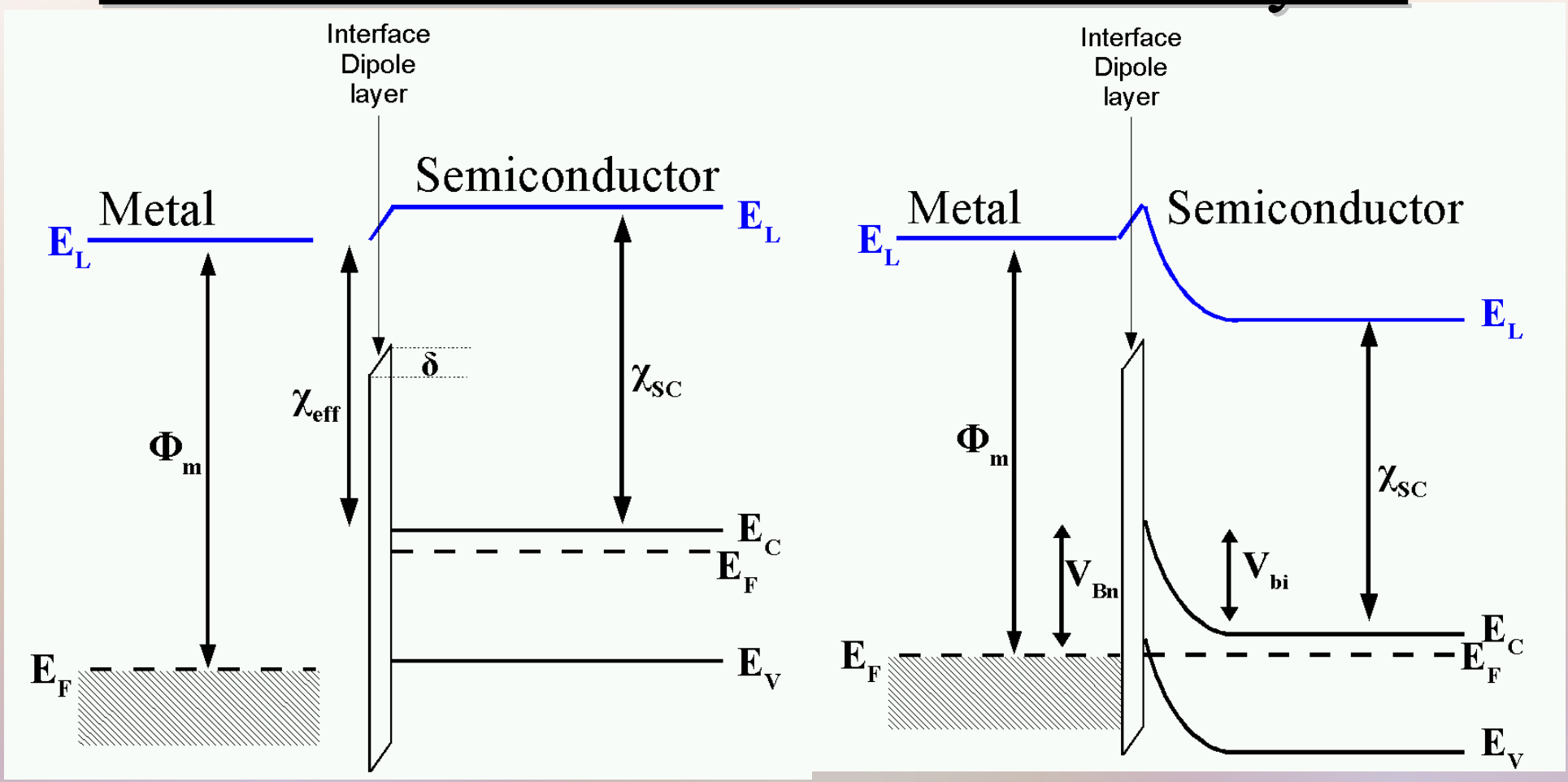
b) Thermal equilibrium



$$\Phi_{Bn} = \Phi_m - X_{SC}$$

But, In real life and especially for Si, it almost never holds

What is the role of the molecular layer?



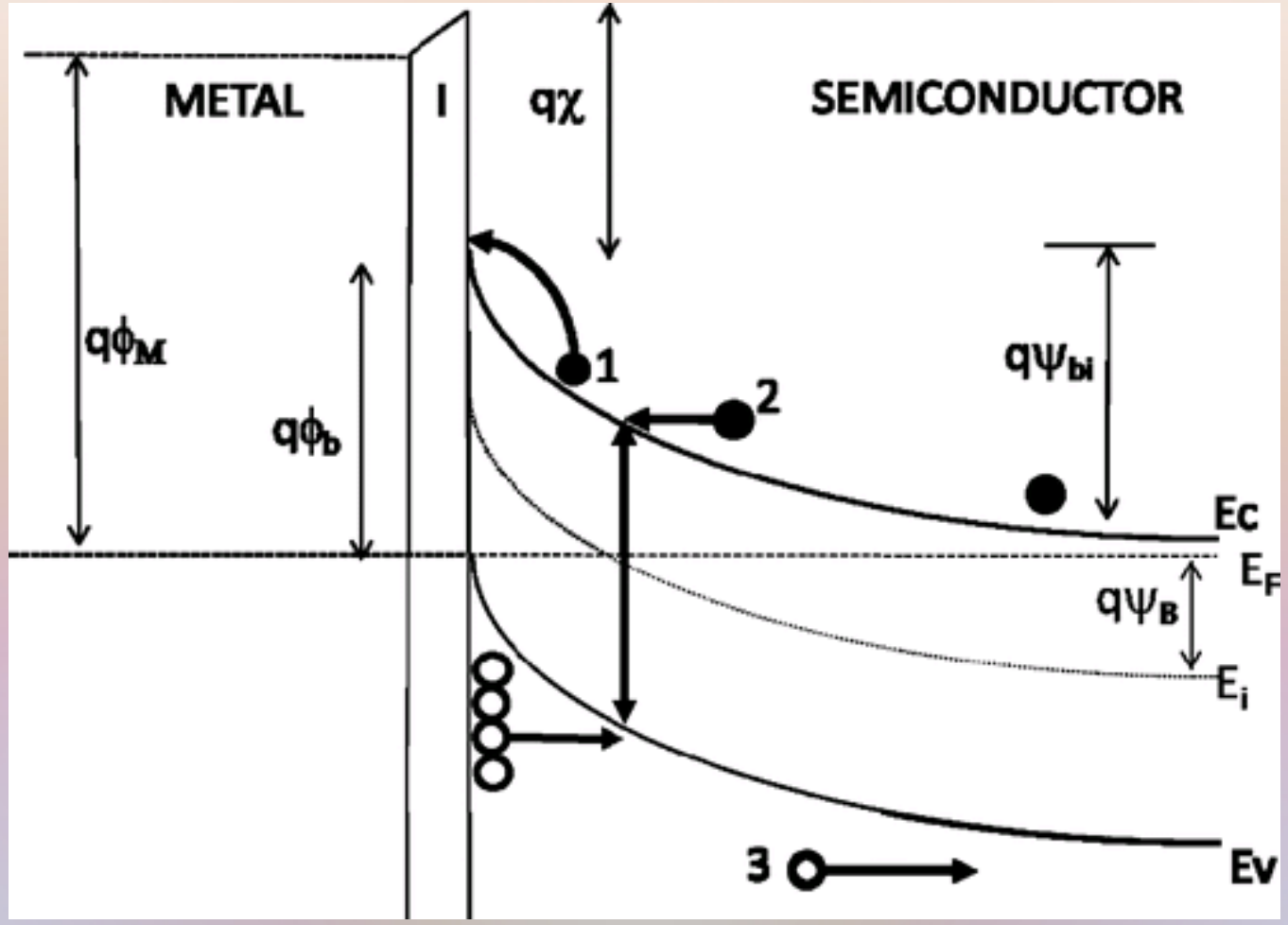
Molecular passivation of the Si decrease surface states density and prevent reaction between the metal and the semiconductor.

Ideal Schottky-Mott behavior

Fortunate coincidence:
Si-C and Si-O-C bonds forms strong negative interface dipole, decreasing effective electron affinity of the Si

$$\Phi_{Bn} = \Phi_m - X_{eff}$$

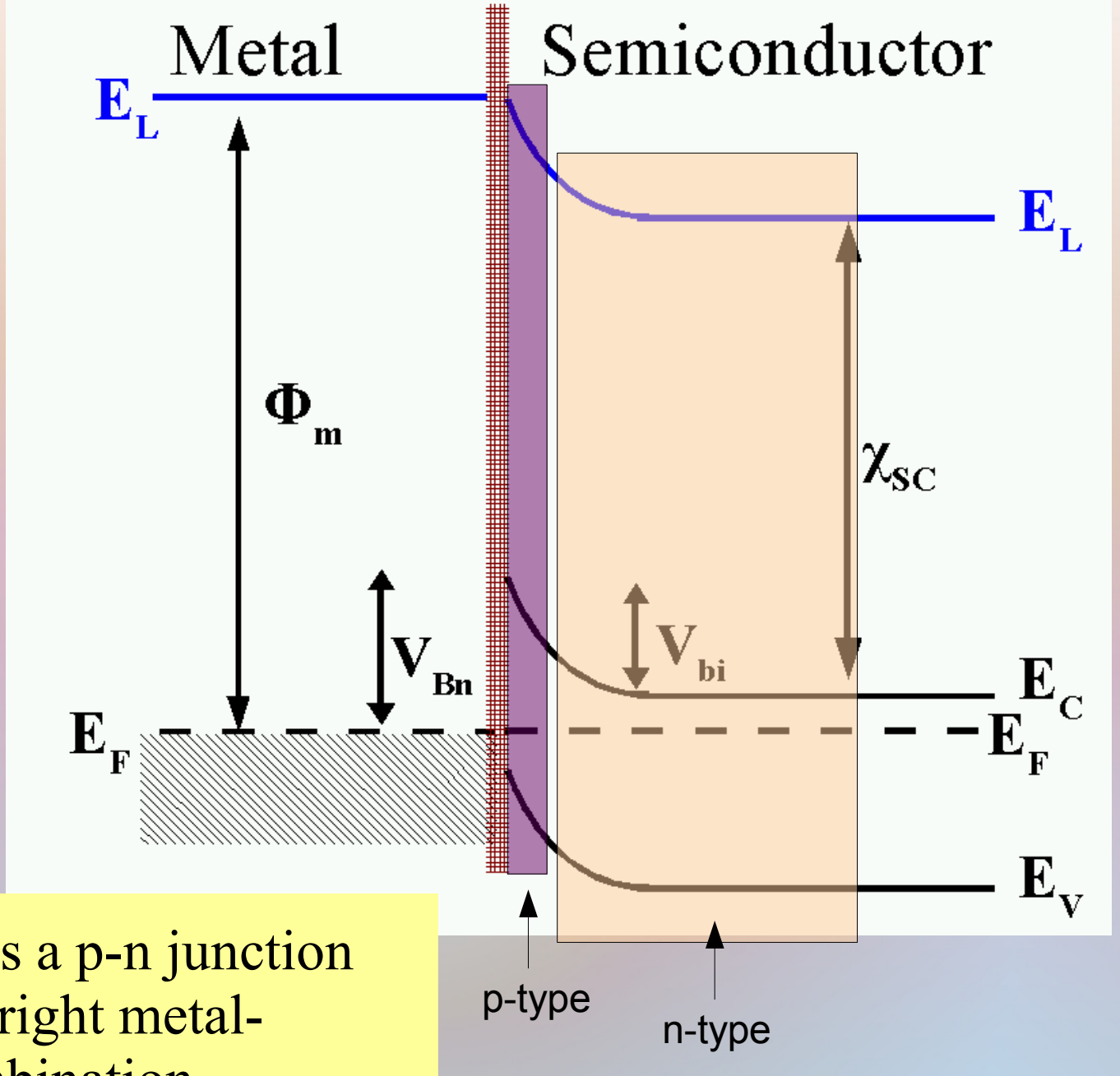
The semiconductor bottleneck



In a fully inverted semiconductor the limiting factors

3. Minority carriers (holes) diffusion in reverse bias
2. Minority carriers (holes) recombination in low forward bias

Inversion layer solar cell (MIS)

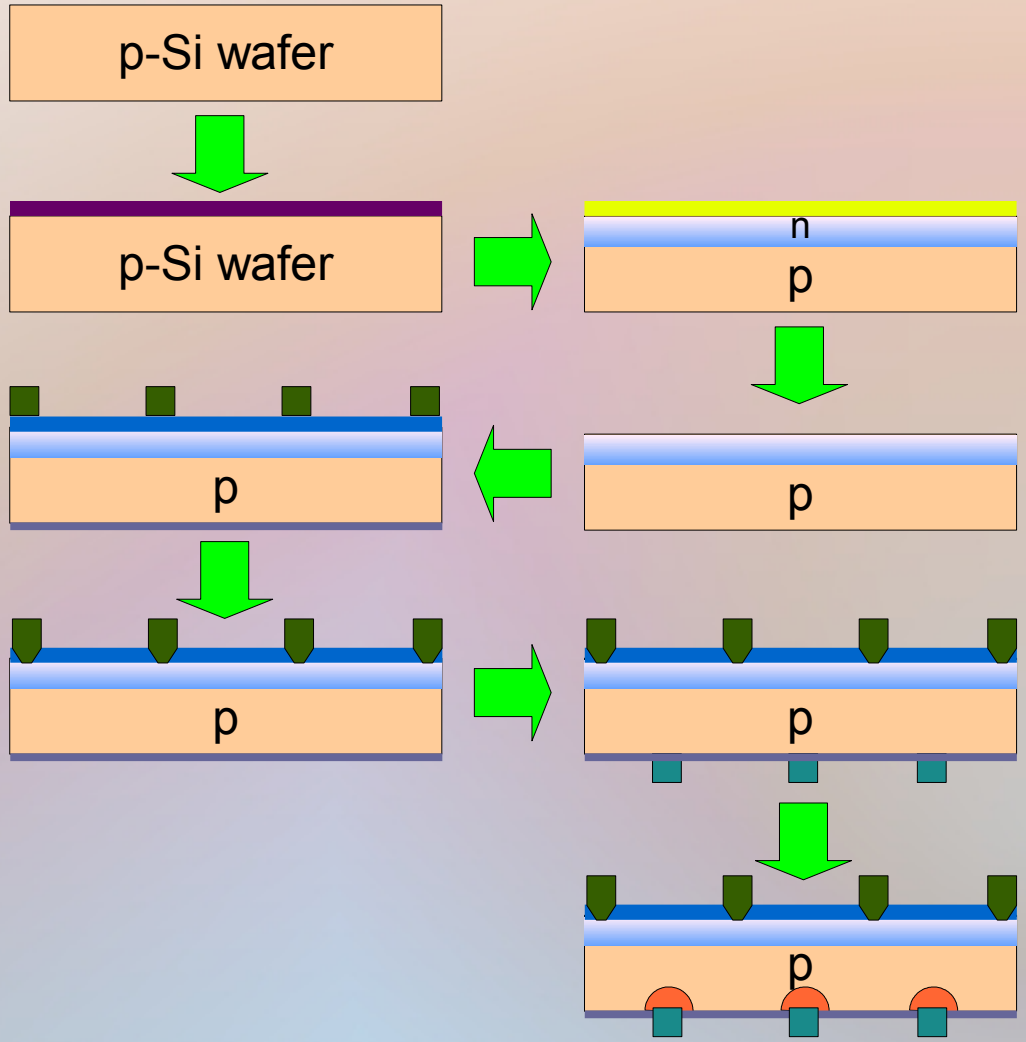


Essentially, one gets a p-n junction just by picking the right metal-semiconductor combination

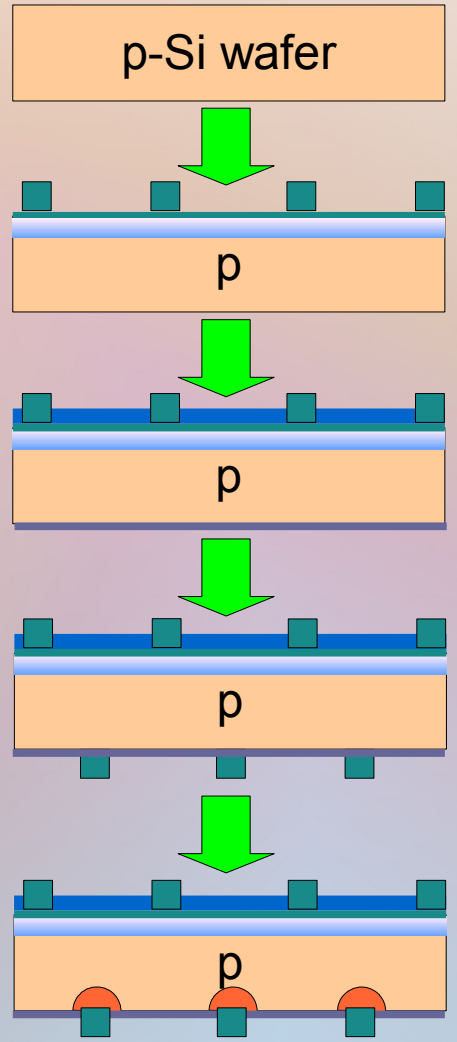
Si inversion layer solar cell process steps

Basically, it is all about process shortcuts

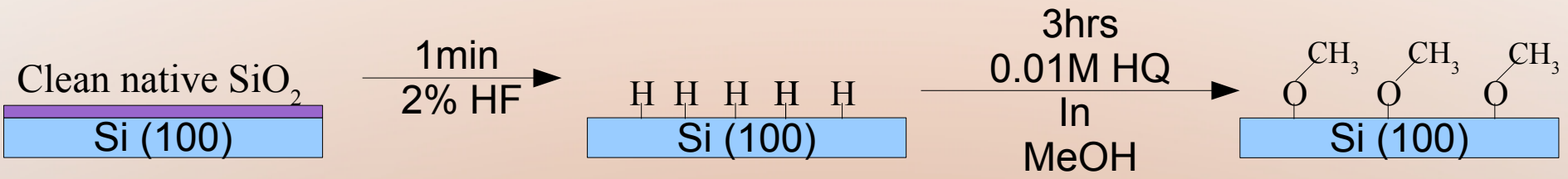
Conventional p-n homojunction solar cell



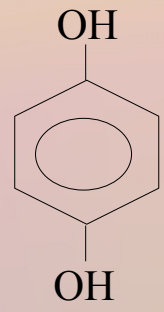
Concept is valid also for n-type absorber



Can we go even milder?



Hydroquinone (HQ):



Takato H. et al, Jpn. J. Appl. Phys., *41, 2002*

Dipole and SPV measurement using vibrating Kelvin probe

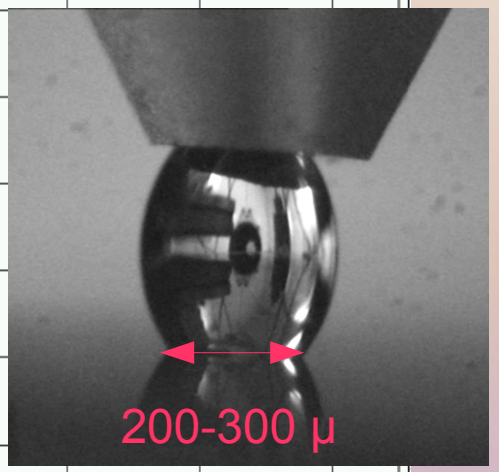
Chemical passivation	Surface photovoltage	CPD* (dipole compared to n-Si-H)	General remarks
Wet HF etching	30-40mV	-530 mV (ref.)	Unstable in air
Thermal alkylation	100-150mV	-850 (-320) mV	Alkylation in ~200°C in air/humidity-evacuated vessel.
Hydroquinone/ MeOH	60-70mV	-1000 (-470) mV	Room-temperature, ambient atmosphere reaction. Stable for (at least) one month in air.

* CPD values are relative to Au reference probe with calibrated work function of 4.7eV

Hg drop top electrode – dark I-V

Recombination current:

$$J_{r0} = \frac{q \cdot n_i \cdot W}{2\tau_r}$$



Abs. Current Density [A/cm²]

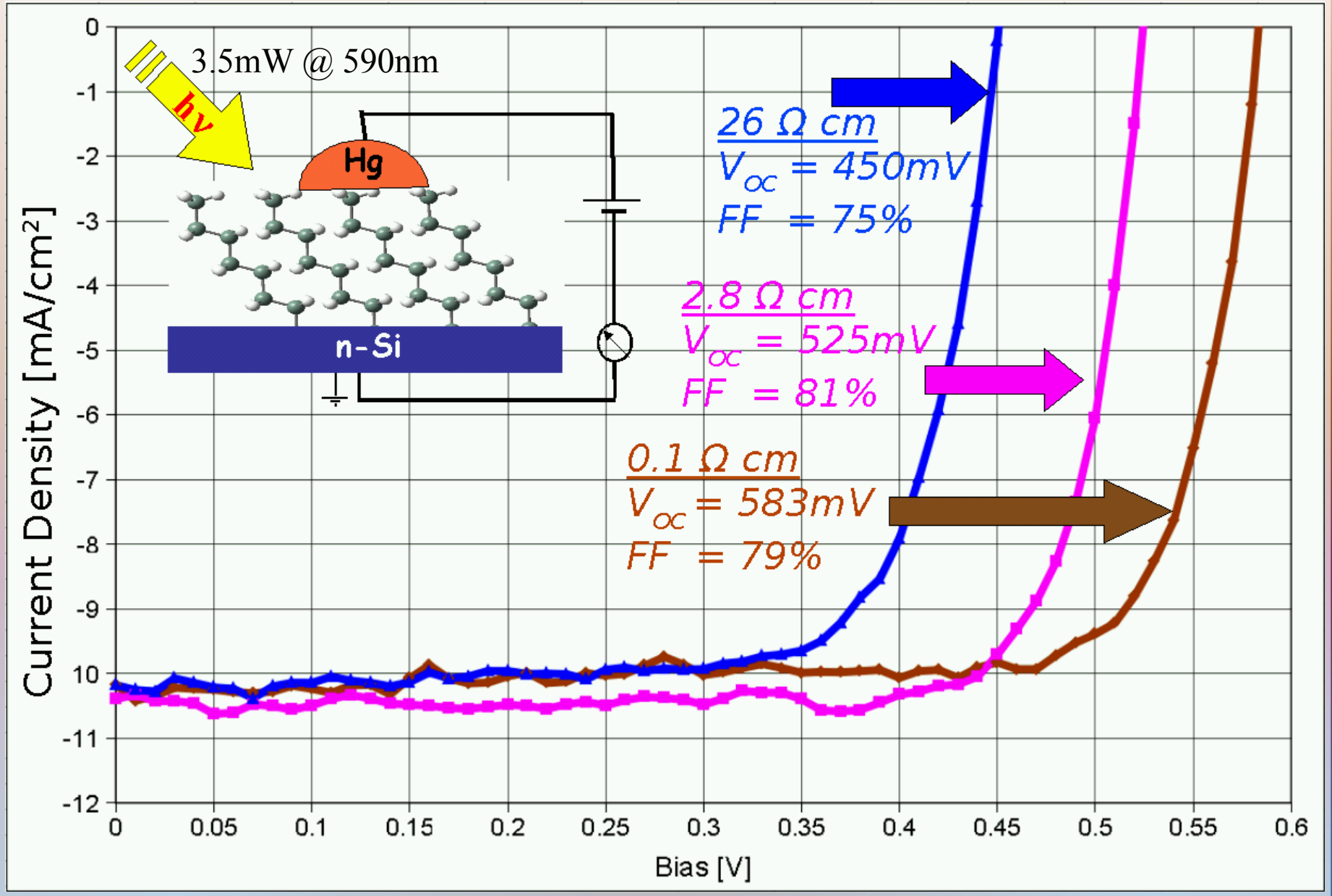
10^{3} 10^{2} 10^{1} 10^{0} 10^{-1} 10^{-2} 10^{-3} 10^{-4} 10^{-5} 10^{-6} 10^{-7} 10^{-8} 10^{-9} 10^{-10} 10^{-11}

-1.0 -0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0 1.2

Bias [V]

0.1 Ohm cm
2.8 Ohm cm
26 Ohm cm

PV under yellow laser illumination



Summary

1. Methanol/hydroquinone treatment is demonstrated as a simple way to passivate Si surfaces.
2. An additional molecular dipole of 0.5V compared to Si-H was measured using vibrating Kelvin probe measurements
3. Upon contact with Hg drop top electrode, Si surface is fully inverted:
   - dark I-V is dominated by minority carriers recombination.
   - The V_{OC} in the photovoltaic measurements is governed by the sample's initial doping density.
4. This treatment can be used as a first step en route to n-Si inversion layer solar cell, using high work function, transparent top electrode.

Thank You