Heterojunction Based Hybrid Si Nanowire Solar Cell

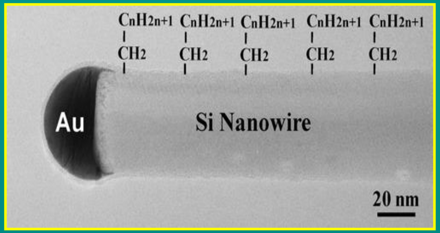
Muhammad Y. Bashouti

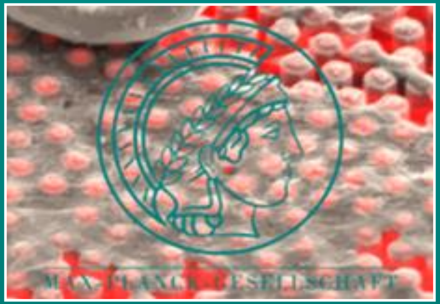
Alexandre Yersin Department of Solar Energy and Environmental Physics

Sde Boqer Campus, BGU

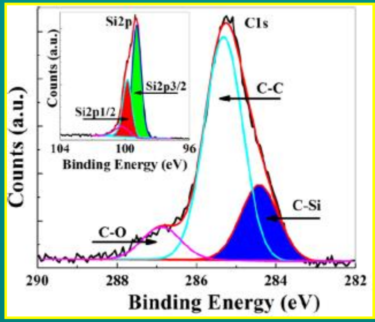
Material Growth

Surface Engineering

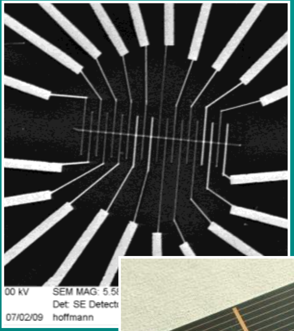




Characterization



Devices prototype



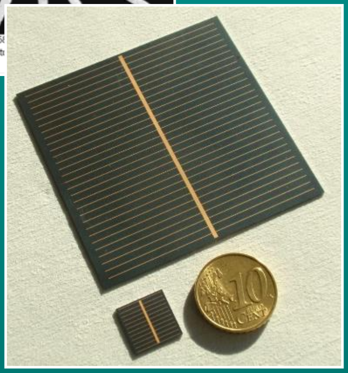


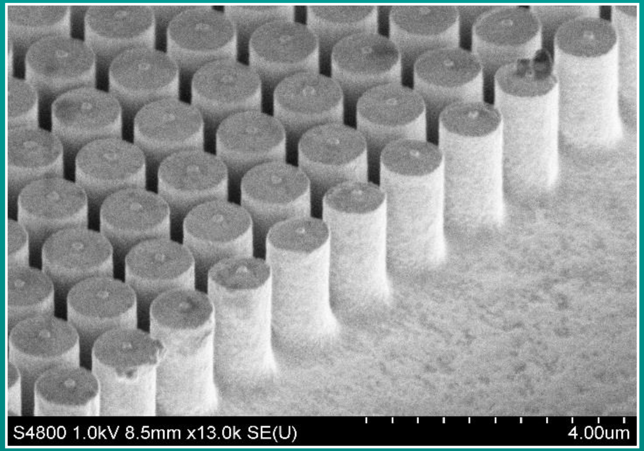
Table of Contents

Introduction

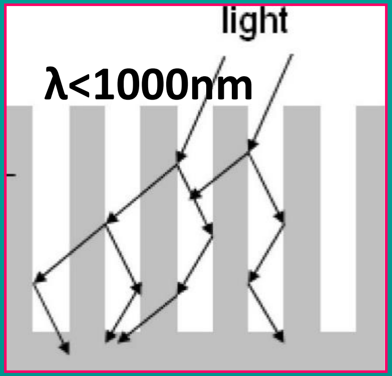
Important features of Nanowires
Obstacles
Molecules

Important features of Nanowires

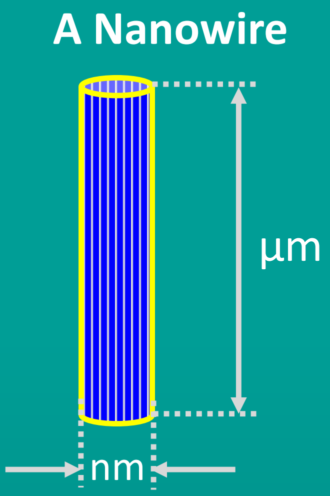
- They represent the smallest efficient transport
- Increased surface scattering
- Orthogonal Junction

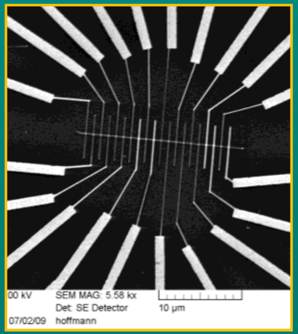


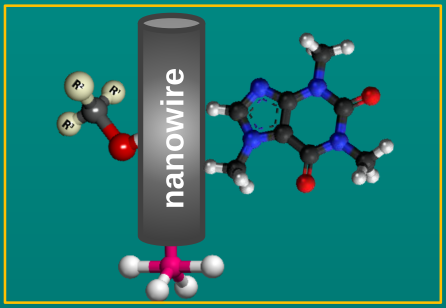
- Increased surface area
- Integration & Devices



Reflection ~<10%



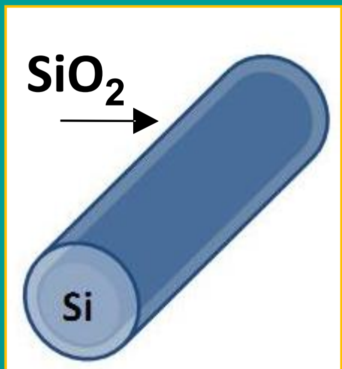




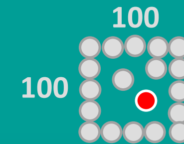
Obstacles on the Road

Obstacles for nanowire growth and surface modifications:

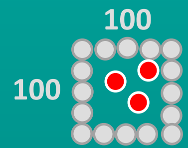
Native oxides



Lowest surface densities ever reported with thermal oxides! ~10^{10} cm^{-2} (Si surface density ~10^{14} cm^{-2}). However:



Amorphous oxides: (i) Dangling bonds



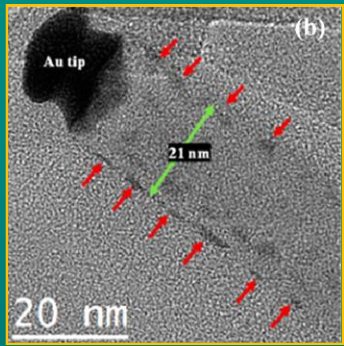
(ii) Induces trap states at the SiO_2/Si interface

(iii) Limits the effect of gate voltage

(iv) No direct chemistry with Si

N. Lewis at. el. *JACS*, (2006): 128, 8990-8991.

Gold diffusion



Gold can behave as an catalyst. However:

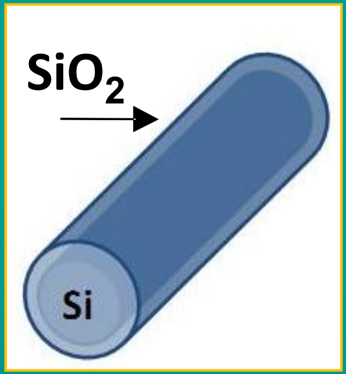
(i) has a high diffusion coefficient 10^{-6} cm^{-2}sec (10^{-9}-10^{-14}) at 1100°C

(ii) Induces deep states inside the band gap

H. Haick, at. el. *ACS Appl. Mater. Interf.* (2012): 4, 4251.

Obstacles for nanowire growth and surface modifications:

Native oxides



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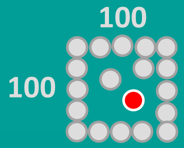

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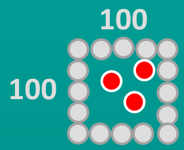

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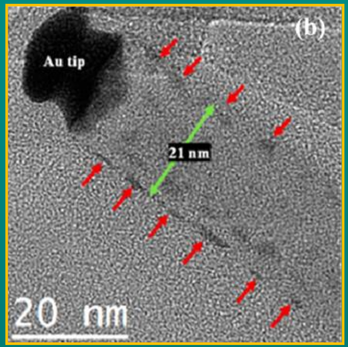
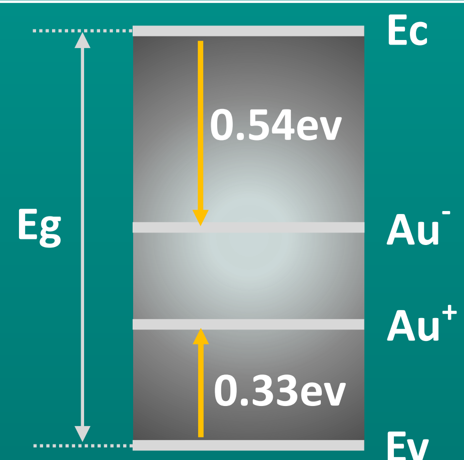
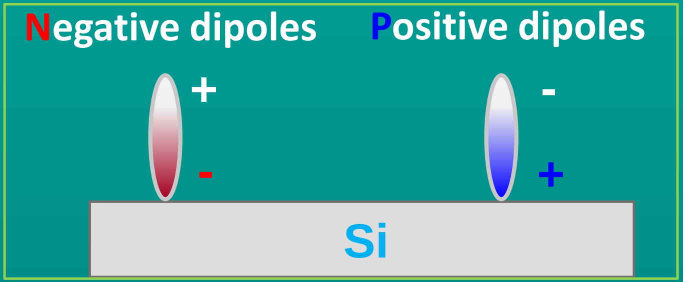


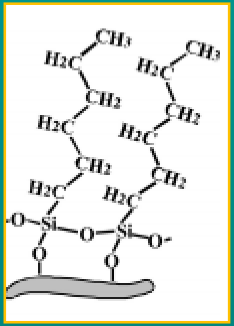


Advantages of using Molecules

- **A promising approach to overcome the aforementioned obstacles is to use molecules. Main advantages are as follows:**

  - Terminating dangling bonds → low surface state density
  - Systematic dipoles → (work function design, surface dipoles)





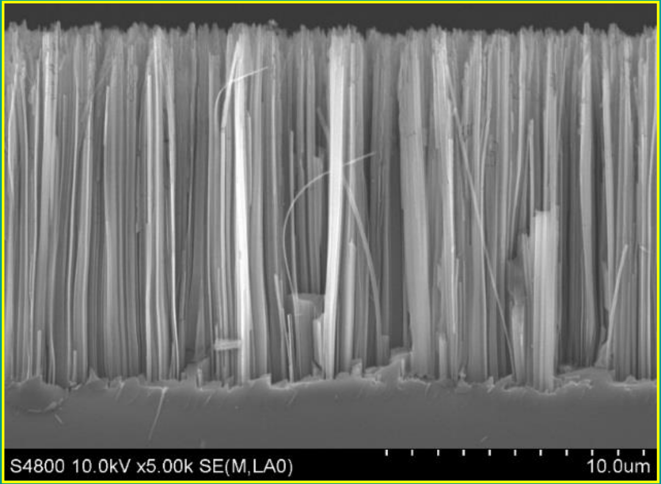
  - Controlling the molecular density
  - Controlling cross-linking
  - Stabilizing the surface (superior oxidation resistance)
  - Molecular surface transfer doping: Controlling the doping level and type (p or n) through organic molecules.

Chapter 1
Realizing Si Nanowires (Si NWs)

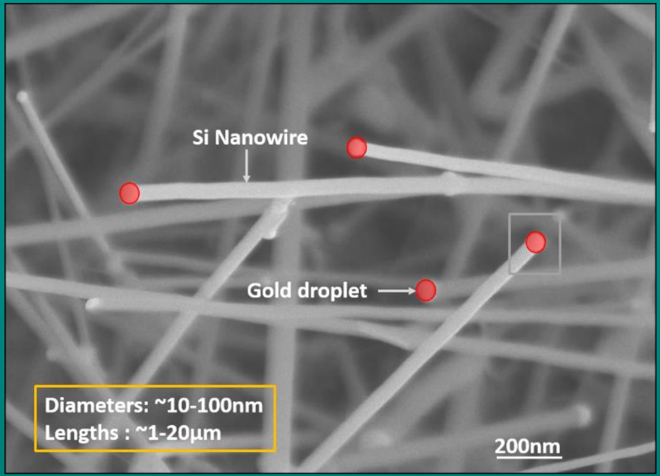
Top Down (Wet and dry etching)

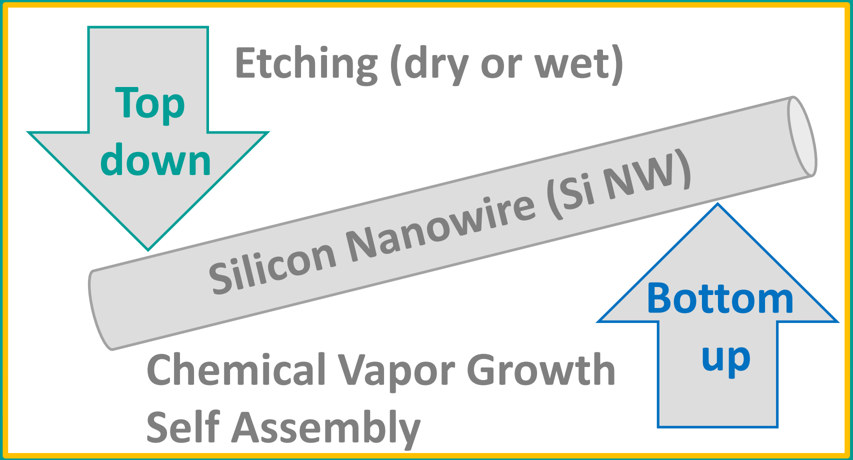
Realizing Si Nanowire: Top down

Top down approach: Wet etching



Bottom Up: CVD process





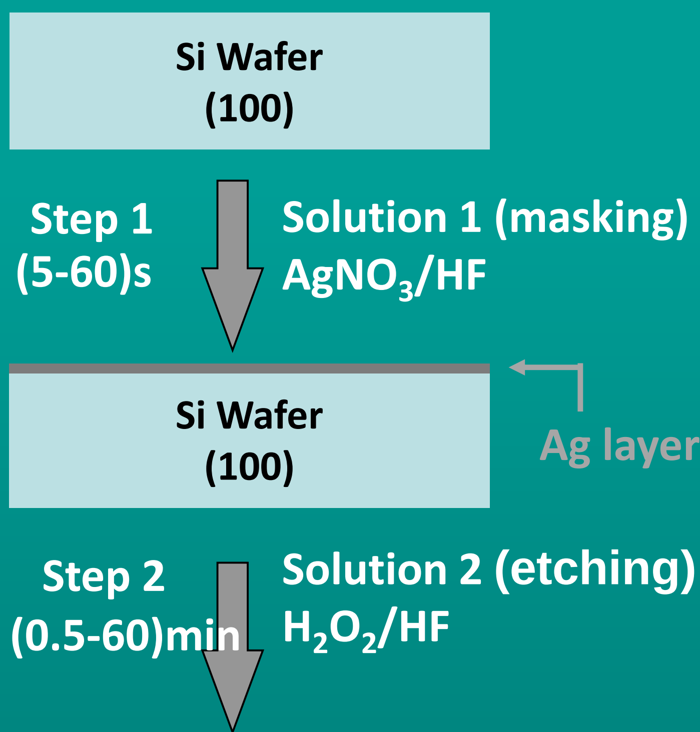
Main Advantages wet chemistry

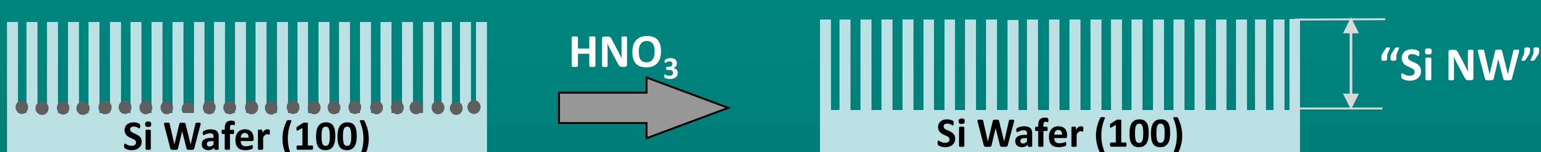
- No need for special equipment's
- Fabricating Si NWs in a few minutes
- Large areas (4 inch)
- High aspect ratio
- Diameter of sub-micro

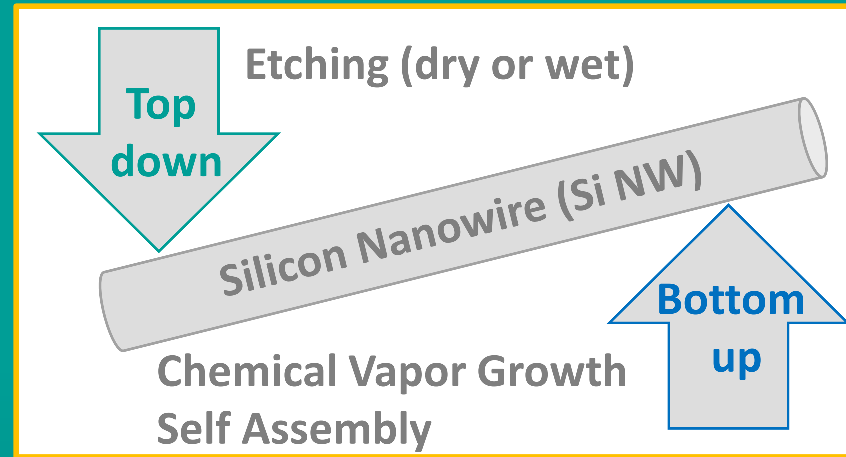
Bashouti, Y. M.; *at. el.* (2013): Progress in Surface Science, 88, 39-60. (Invited Review)

Realizing Si Nanowire

- Top down approach: Wet etching (two step process)







Main Advantages

- No need for special equipment's
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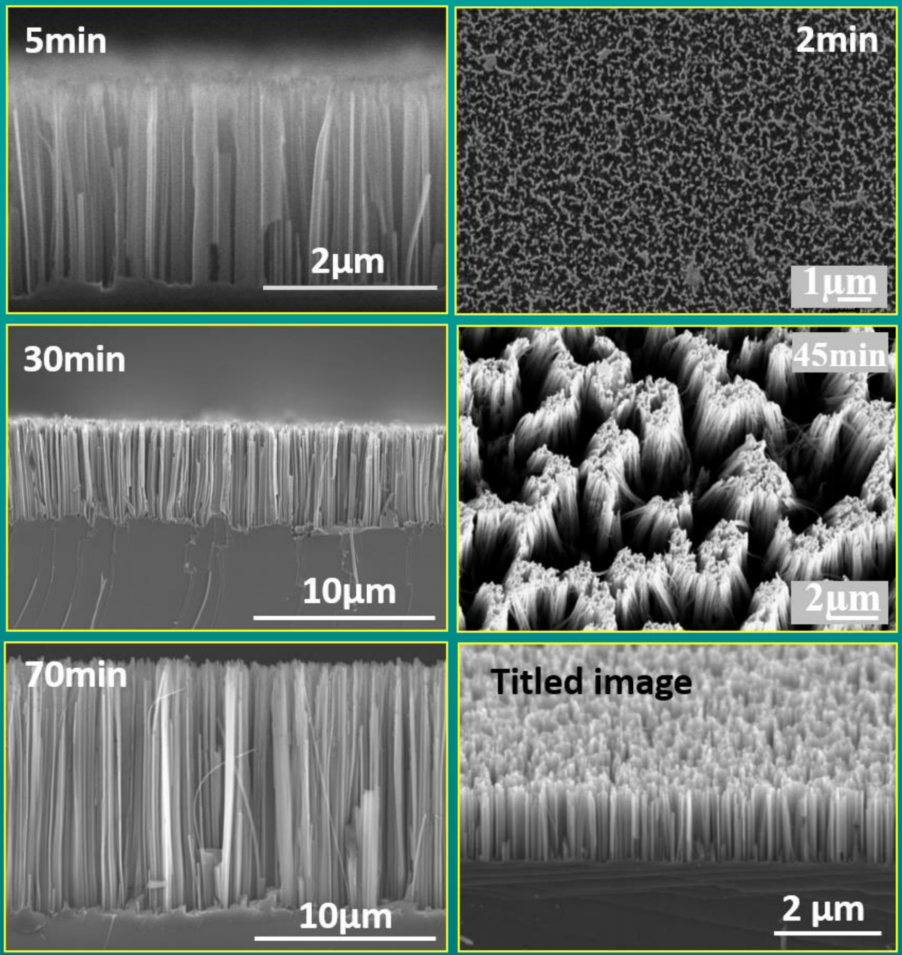
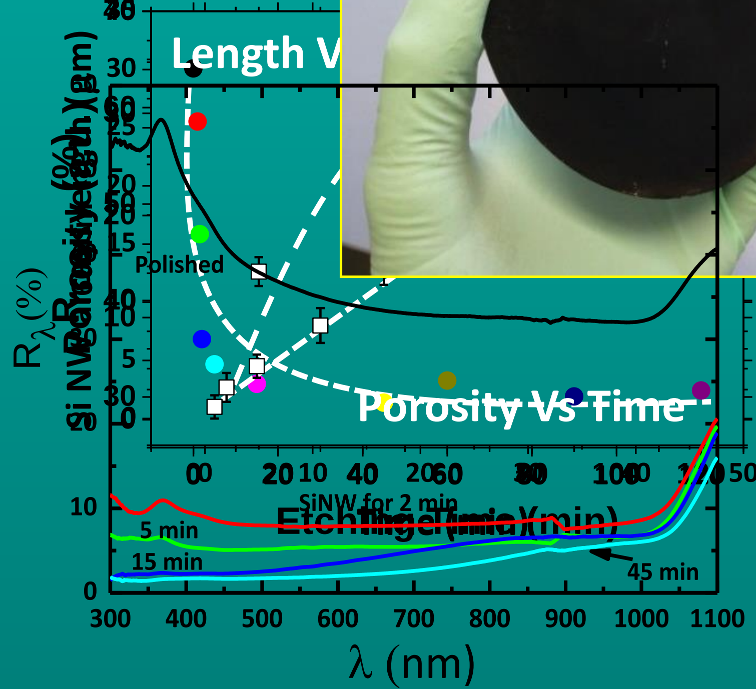
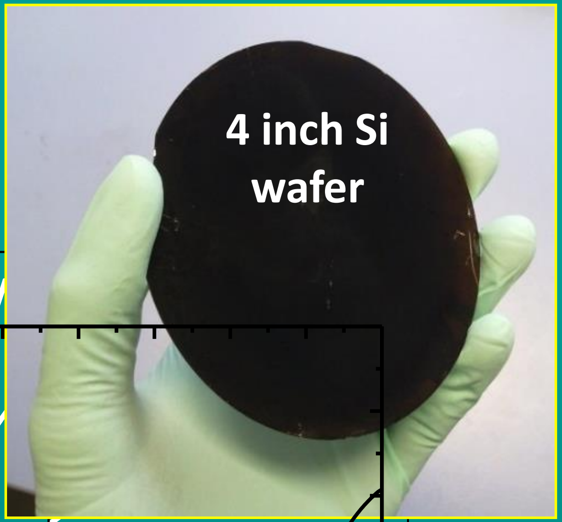
- High aspect ratio

Top down approach: Wet etching
(two step process: step II – Etching time)







Top down approach (wet etching) *Cont.*

- Top down approach: Wet etching (the mechanism)

Nano local electrochemical reaction

Cathode Reaction:

$$4Ag^+ \longrightarrow 4Ag_{(s)} + 4h^+$$

Anode Reaction:

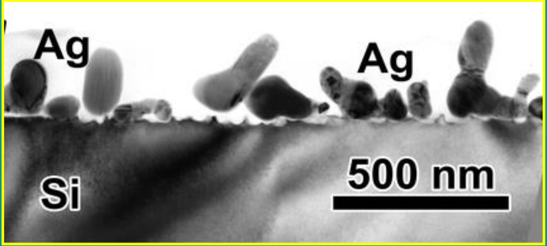
$$Si_{(s)} + 2H_2O + 4h^+ \longrightarrow SiO_2 + 4H^+$$

$$SiO_2 + 4H^+ \xrightarrow{6HF} H_2SiF_6 + 2H_2O$$

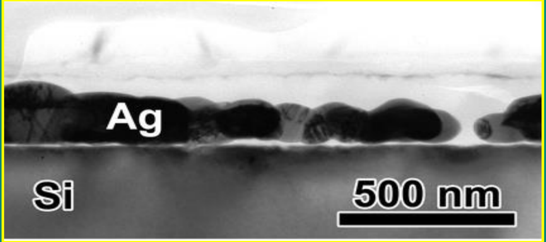
Total Reaction

$$Si_{(s)} + 4Ag^+ + 6HF \longrightarrow 4Ag_{(s)} + H_2SiF_6 + 4H^+$$

(i) 15sec



(ii) 30sec



Top down approach (wet etching) *Cont.*

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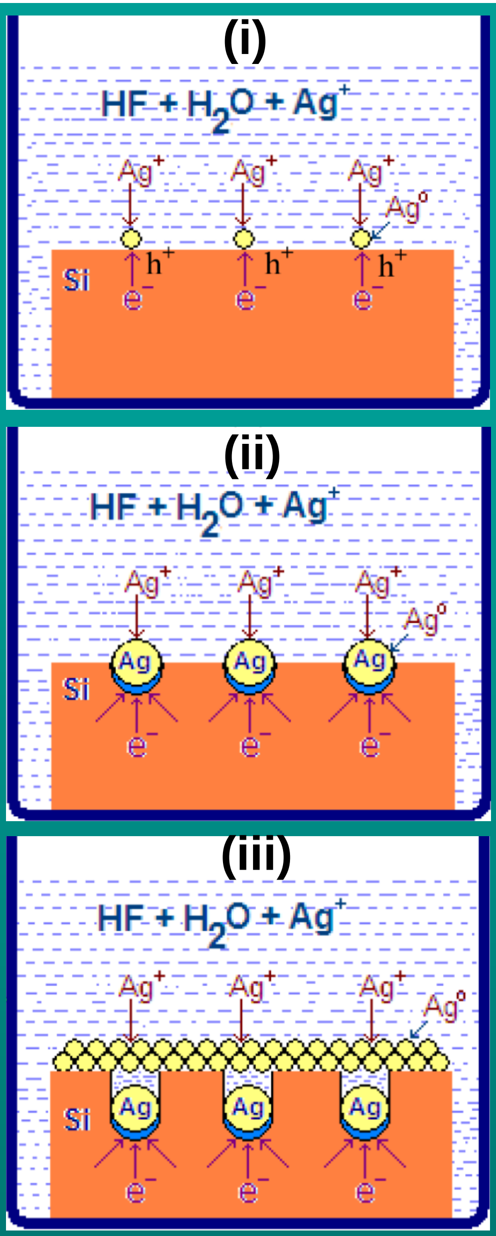
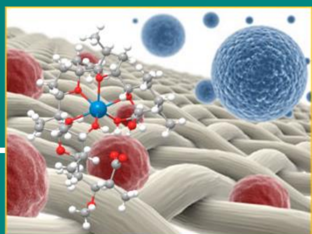


Chapter 2
Surface Treatment & Characterization

Surface Modification

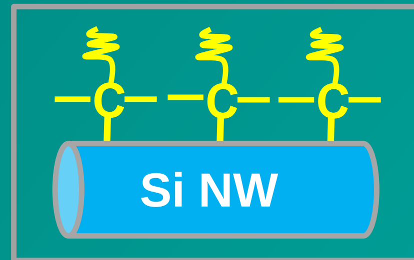


Molecules

Nanoparticles

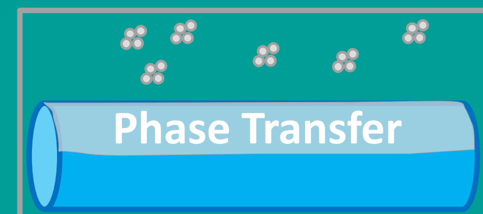
Molecules on Surfaces

(Grignard Reaction, Electrografting)



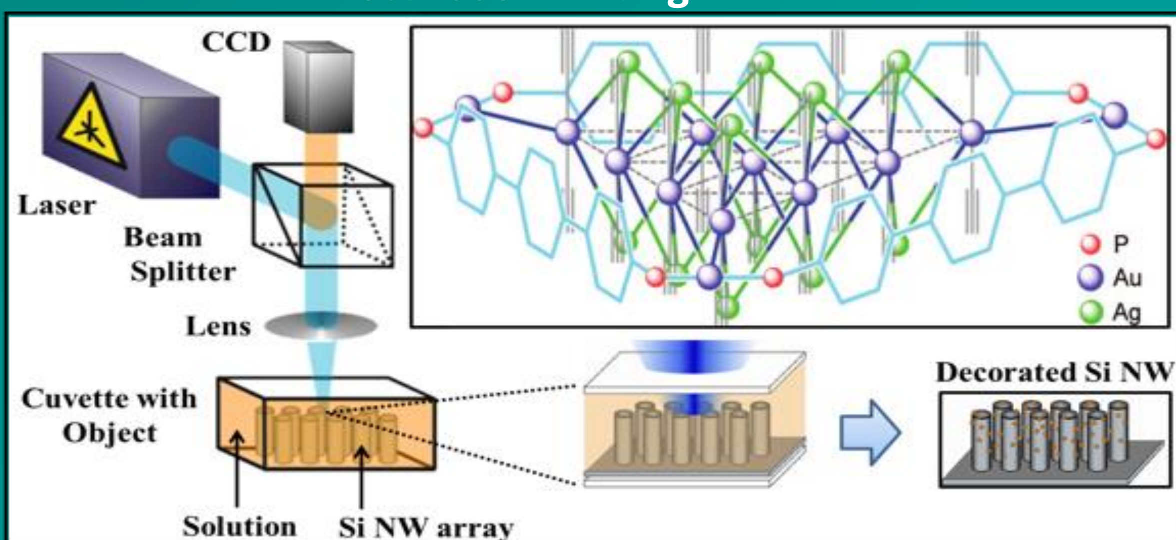
Phase Transfer

(From Cubic to Wurtzite)



Bashouti, Y. M. at el. (2016): Sci. Rep. Accepted

Direct Laser Writing



Bashouti, Y. M. at el. (2015): Lab-on-Chip, 15, 1742-1747. DOI: 10.1039/c4lc01376j

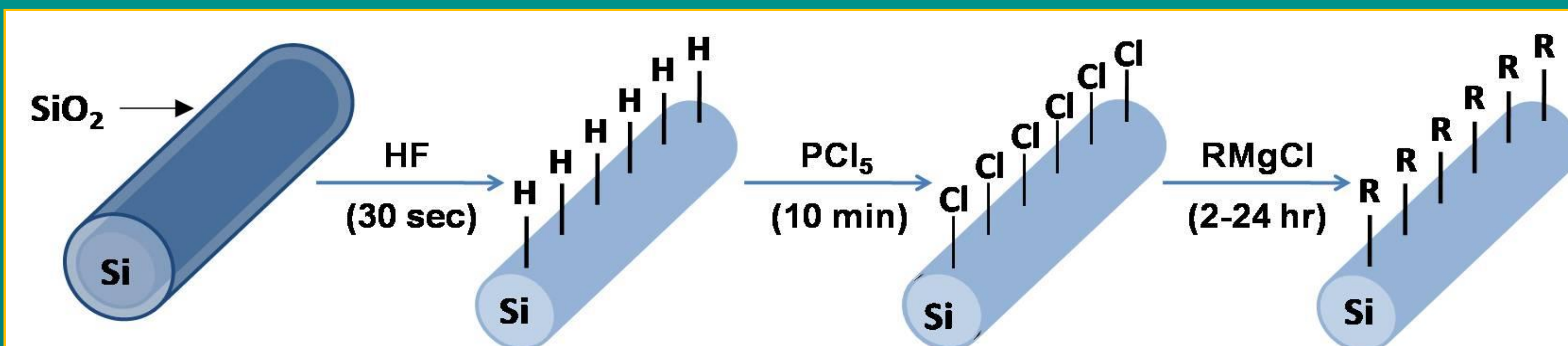
Molecules on Surfaces: Grignard Reaction

Molecules on Surfaces: Grignard Reaction

1) Characterization?
2) Replacing oxide shell?
3) Si-C bonds?
4) Maximum Coverage?
5) Stability?
6) Oxidation Mechanism

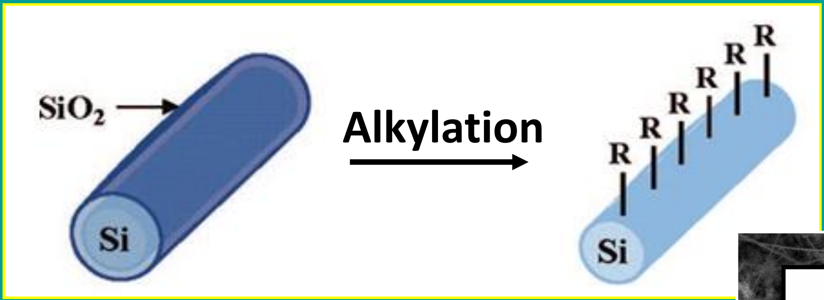
- ✓ Two step chlorination/alkylation process
- ✓ Etching : Removes the native oxide layer (makes H-Si)
- ✓ Chlorination: Replace the H by Cl
- ✓ Alkylation: Terminate the Si-Cl to Si-R

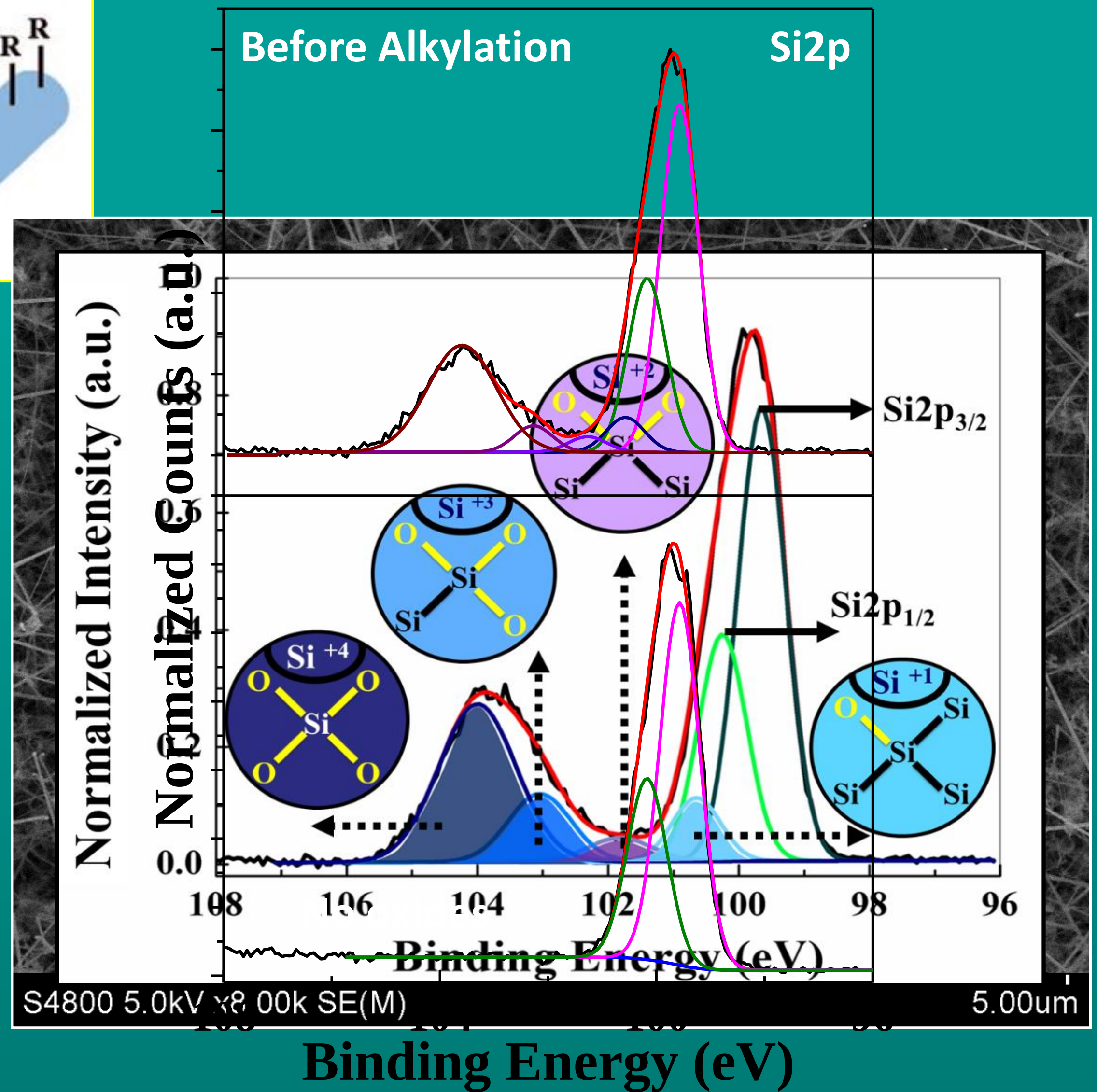
Two Steps Reaction



M. Y. Bashouti, *at. el.* (2008): JPCC, 112, 19168-19172.
M. Y. Bashouti, at. el. (2009): JPCC, 113, 14823-14828.

Si2p & C1s of Terminated Si NW





M. Y. Bashouti, at el. (2012): Phys. Chem. Chem. Phys., 14, 11877-11881.

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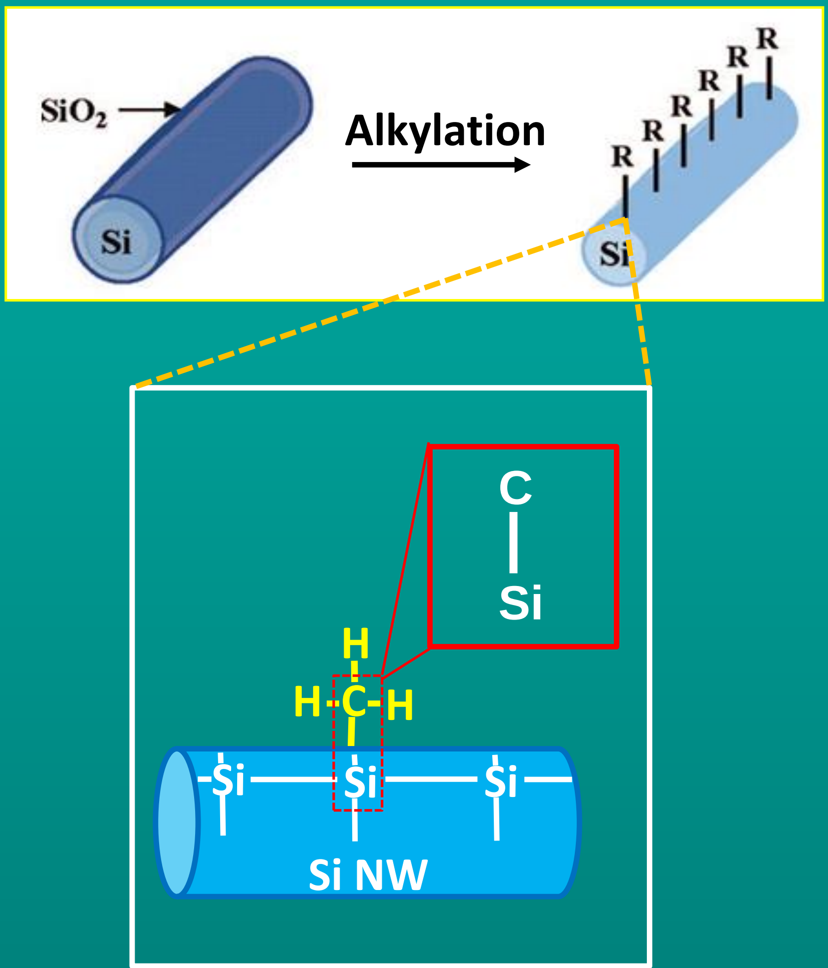
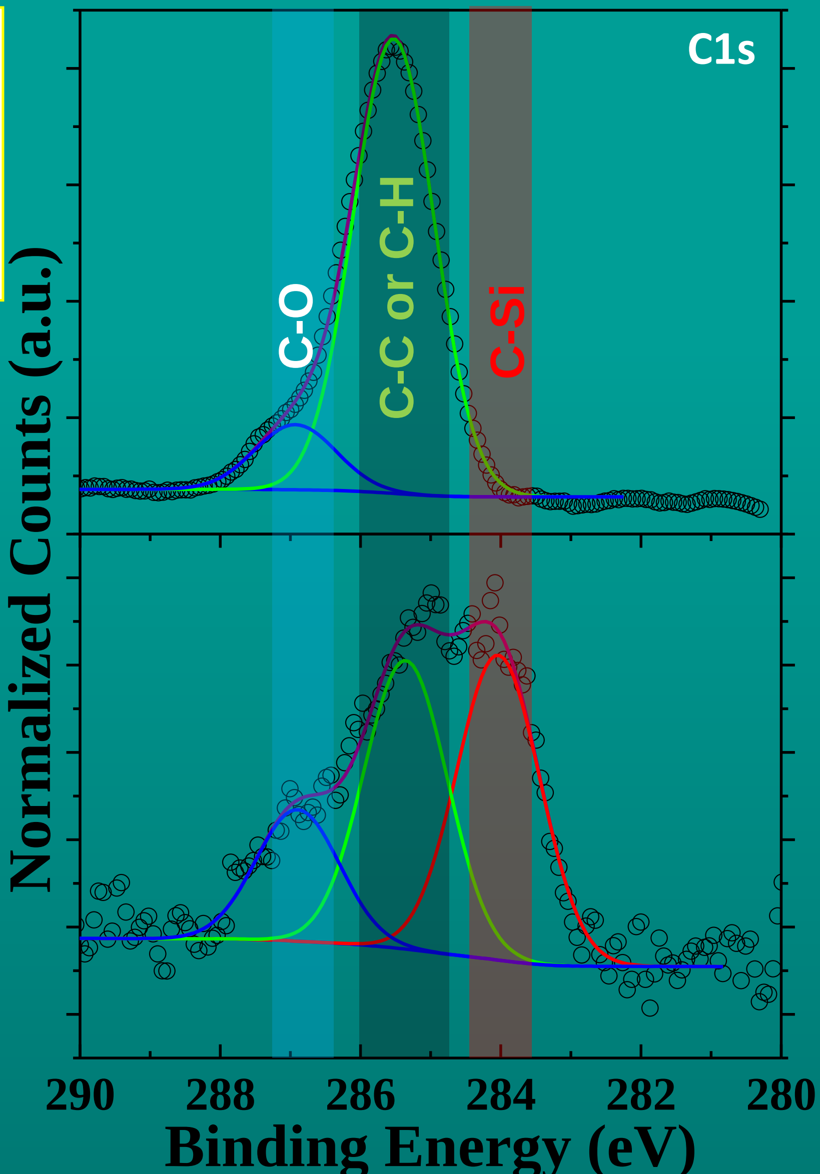


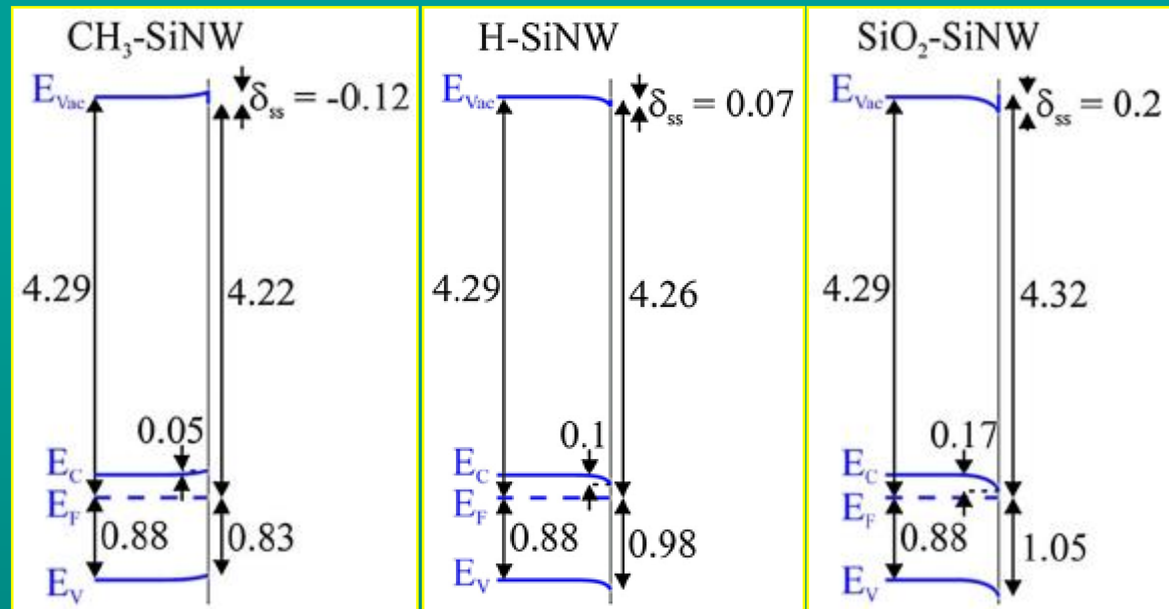


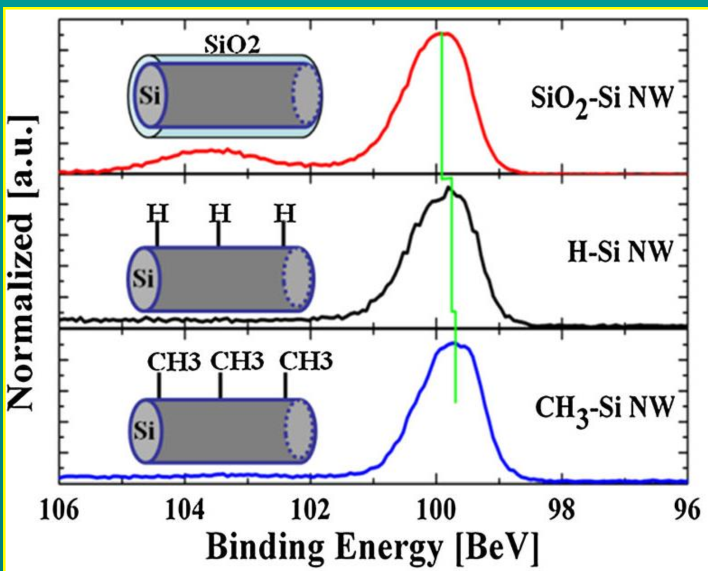
Impact on Density of State (DOS)
In Suite Measurements

We followed the DOS by using the following:

1. **Emission of Si2p**
2. **Photo-electron Yield (PYS)**
3. **Work-Function**

Band diagram of CH_3-SiNW, H-SiNW and SiO_2-SiNW surfaces. All the numbers are in eV unit.





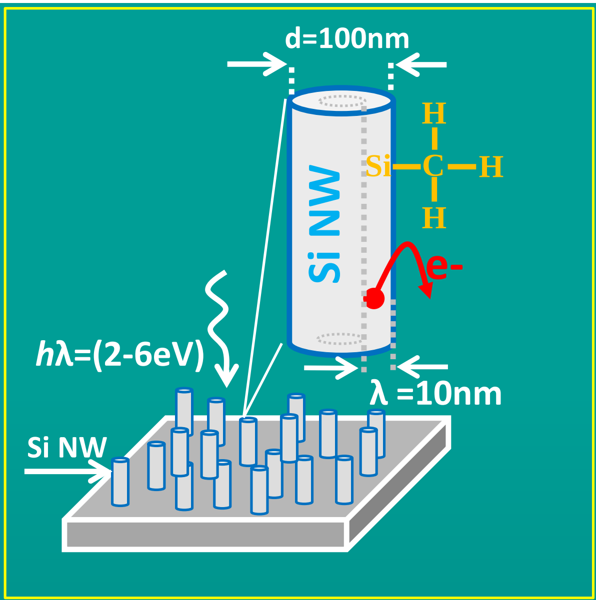
χ_s = Φ-E_g+ (E_F-E_V)

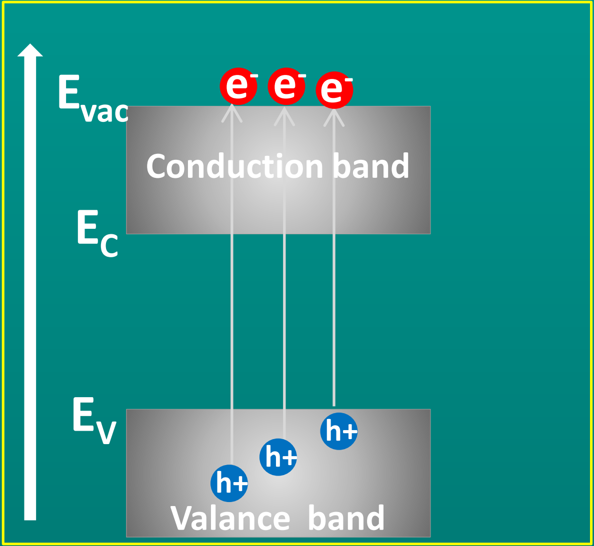
$\delta = \chi_s - \chi_B$

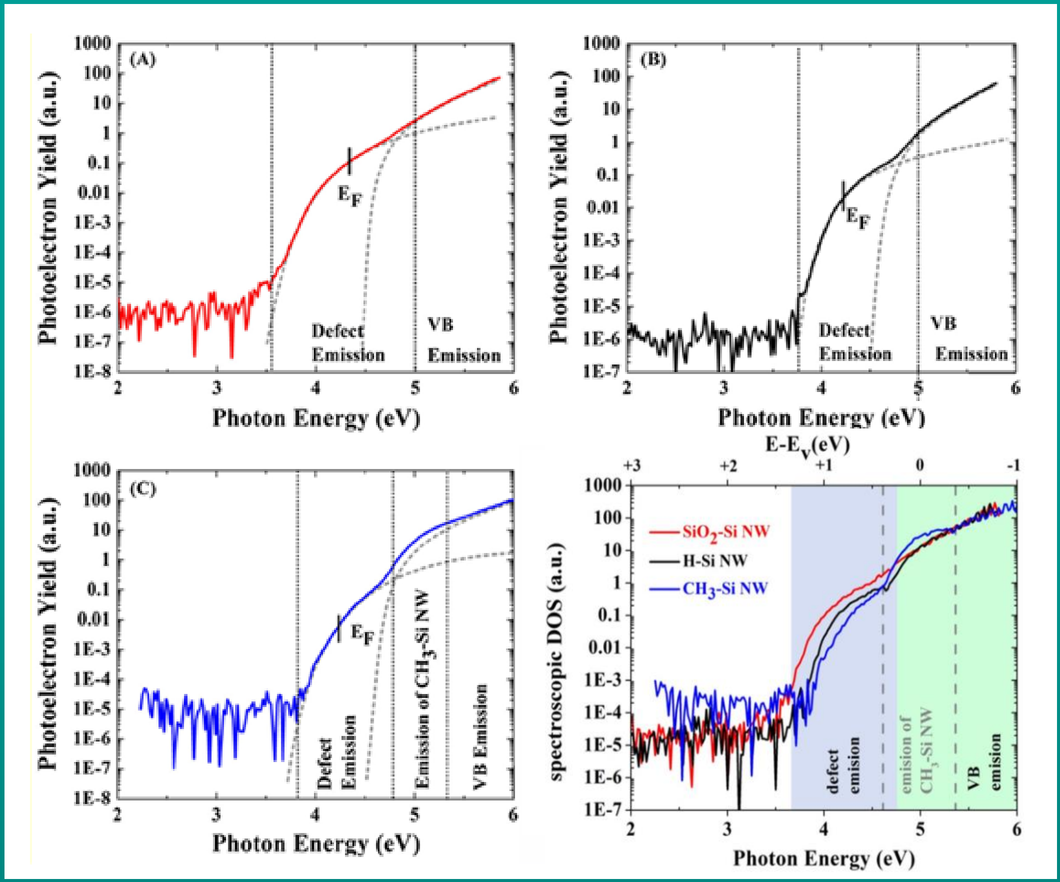
	Si2p	EF-EVBM	Φ
SiO2	99.77	0.83	4.32
H	99.70	0.98	4.26
CH3	99.55	1.05	4.22

M. Y. Bashouti *at. .el. (2014): Prog. Photovolt: Res. Appl.* 2, 1050-1061.

Photoemission of Hybrid Si NW







$$g_{oc}(E_{VL} - \hbar\omega) \propto \frac{dY}{d(\hbar\omega)}$$

g_{oc}= occupied density of states

E_{VL} = Vacuum Level

ħw = optical excitation

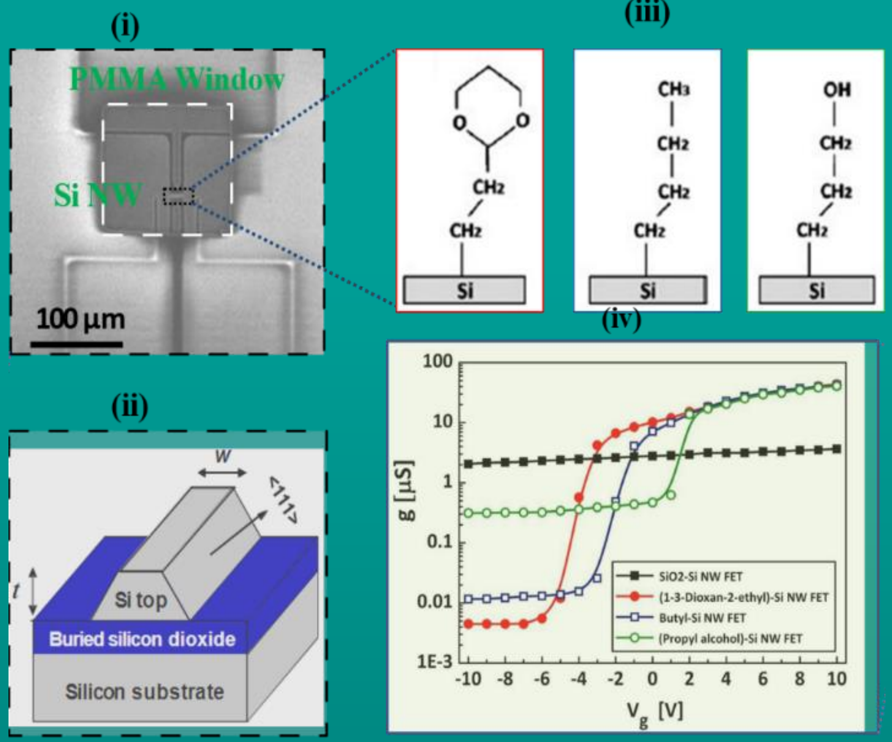
Chapter 3: Devices Solar Cells

Projects: Brief Summary

- **Surface modifications**

  Devices: FETs, Solar Cells, Diodes & Transparent electrodes

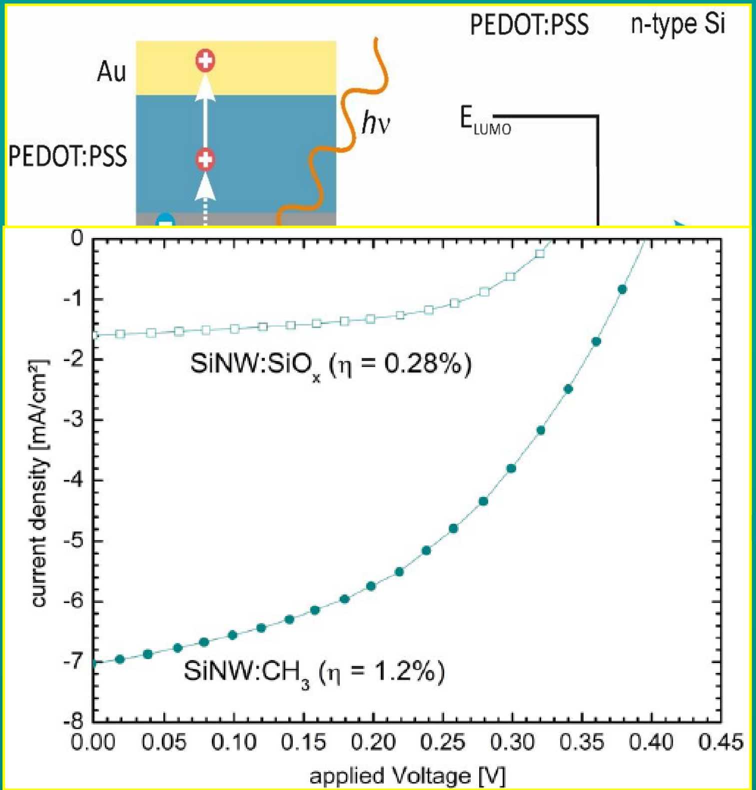
devices: FET

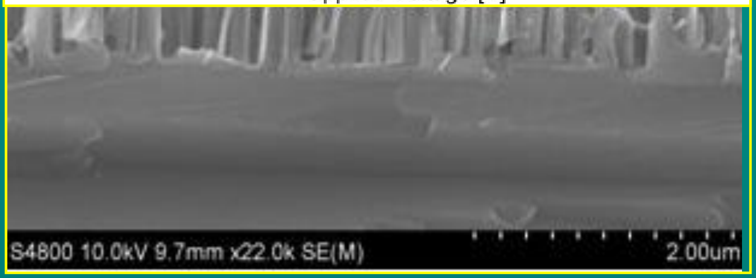


Publications:

1. M. Bashouti, et al. (2009): *Small*, 88:39-60. 5:2761-2769
2. M. Bashouti, et al. (2015): *J. Phys. Chem. Lett.*, 6:3988–3993.
3. M. Bashouti, et al. (2015): *ACS Appl. Mater. Interfaces*, 7: 21657–21661.
4. M. Bashouti, et al. (2016): *Scientific Reports.* (Accepted).
5. M. Bashouti, et al. (2016): *J. Mat. Chem.* (Under revision).

Hybrid Solar Cells: PEDOT:PSS/ Si NW





M. Bashouti, et al. (2014): *Prog. Photovolt: Res. Appl.* 2, 1050.
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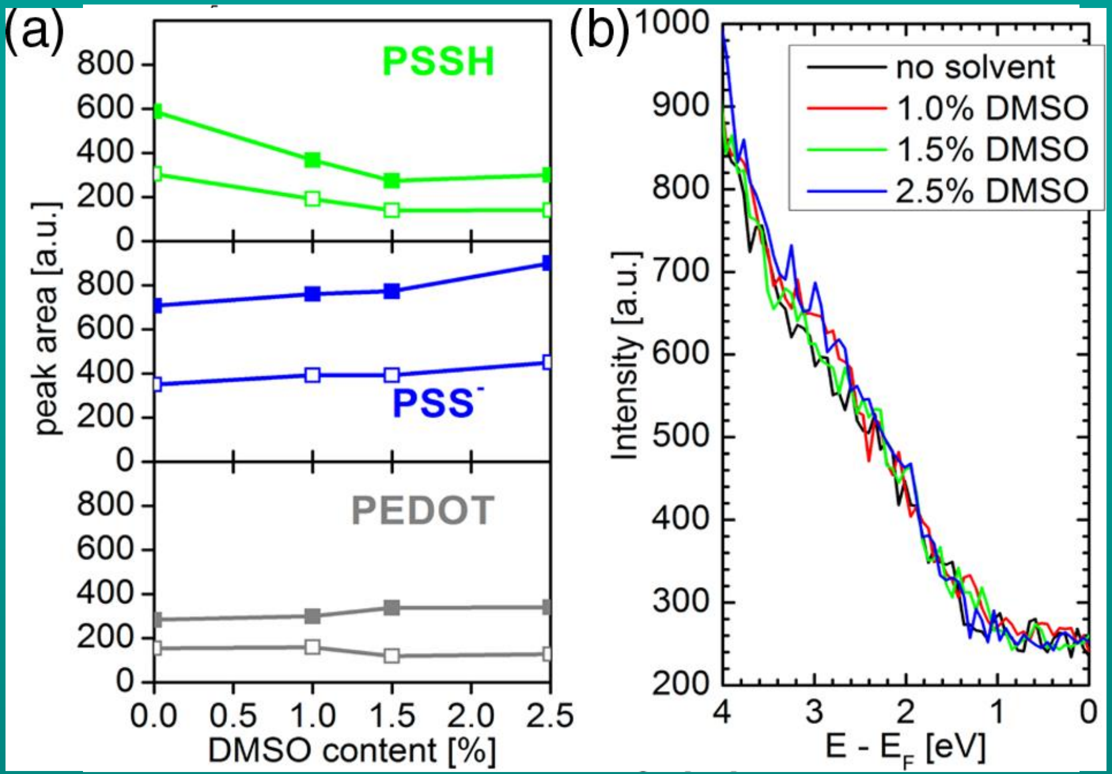

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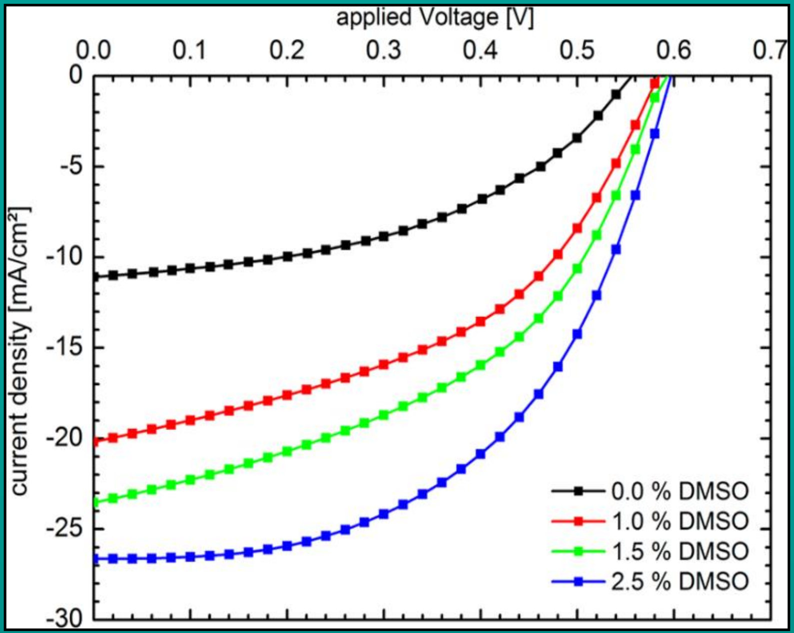

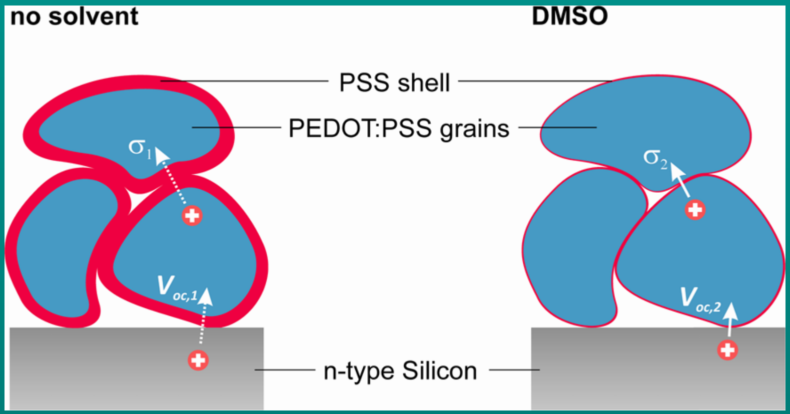

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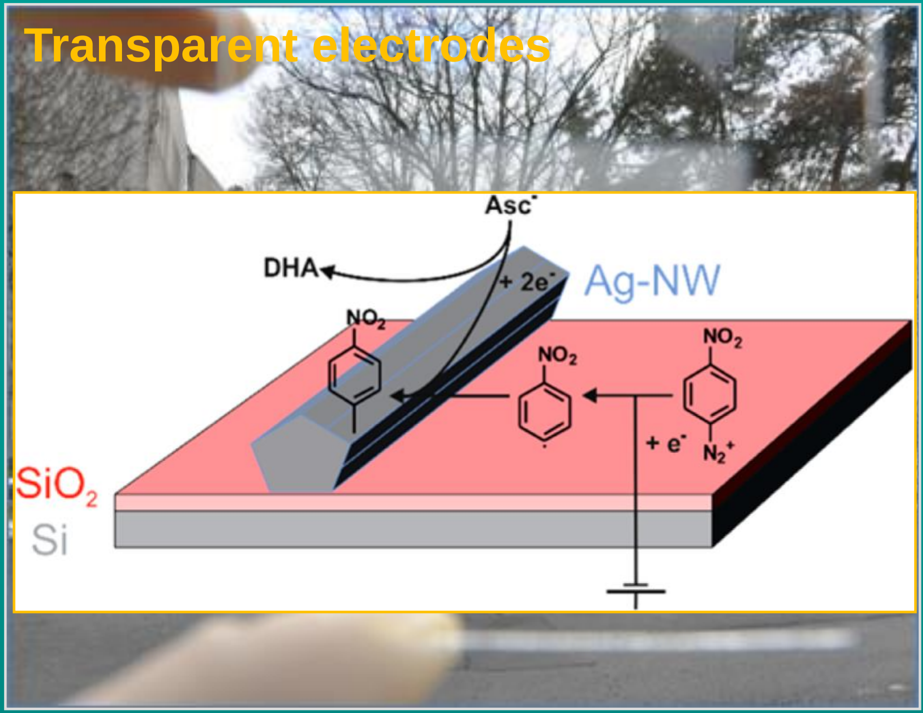
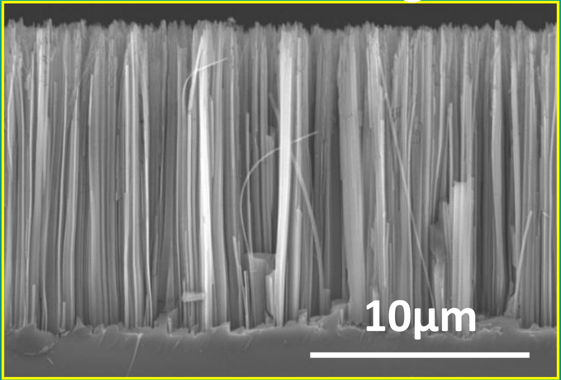


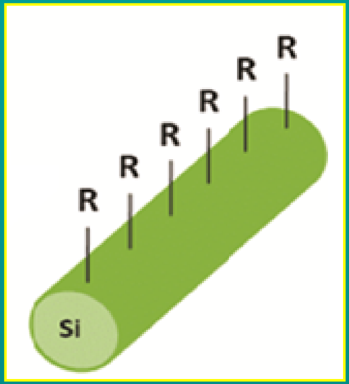
M. Bashouti, et al. (2015): *ACS Appl. Mater. Interfaces*, 7: 21657−21661.
M. Bashouti, et al. (2016): *Langmuir,* (Under revision).

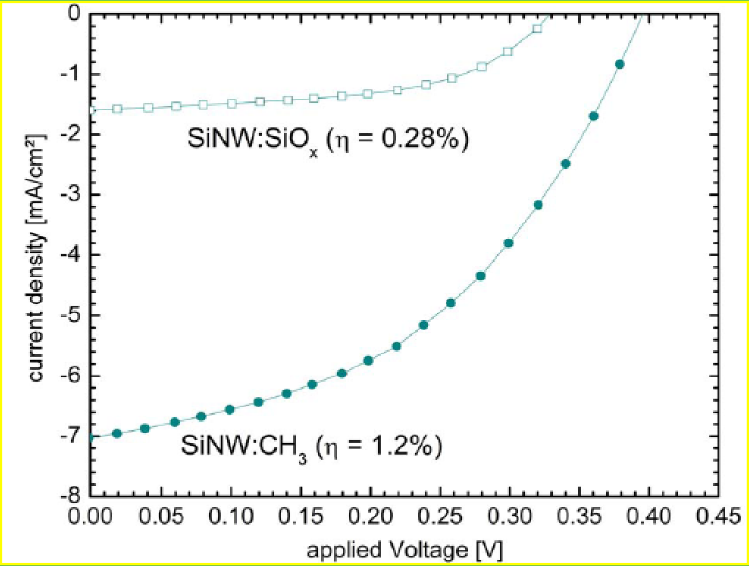
Summary

Wet etching



Termination





Thank you for your attention!