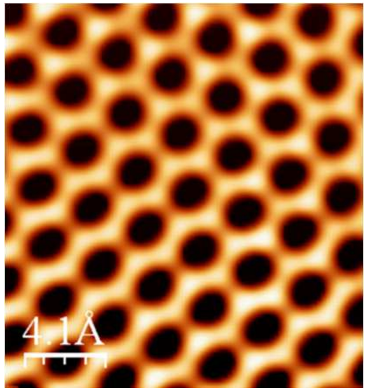
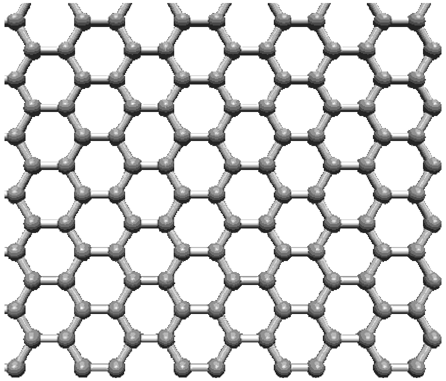
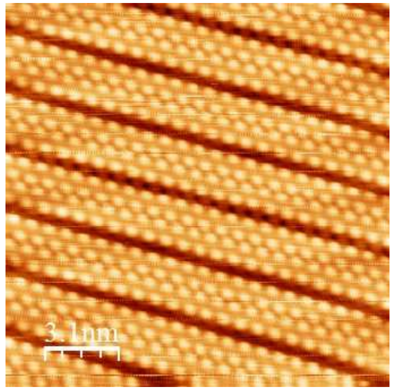
SILICENE: The silicon counterpart of Graphene







Hamid Oughaddou

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Département de physique, Université de Cergy-Pontoise, 95000 Cergy-Pontoise, France

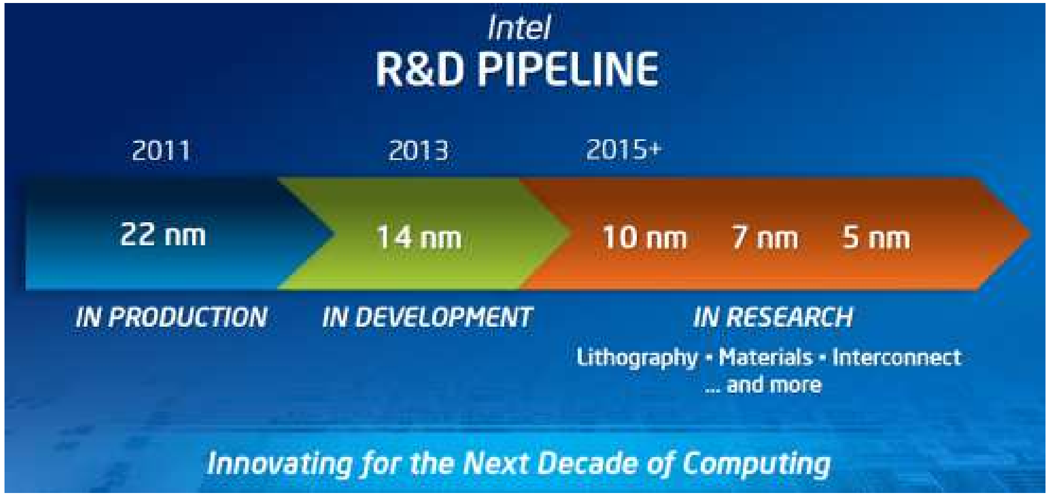
Introduction

“History does not repeat itself, but it does rhyme”

Mark Twain

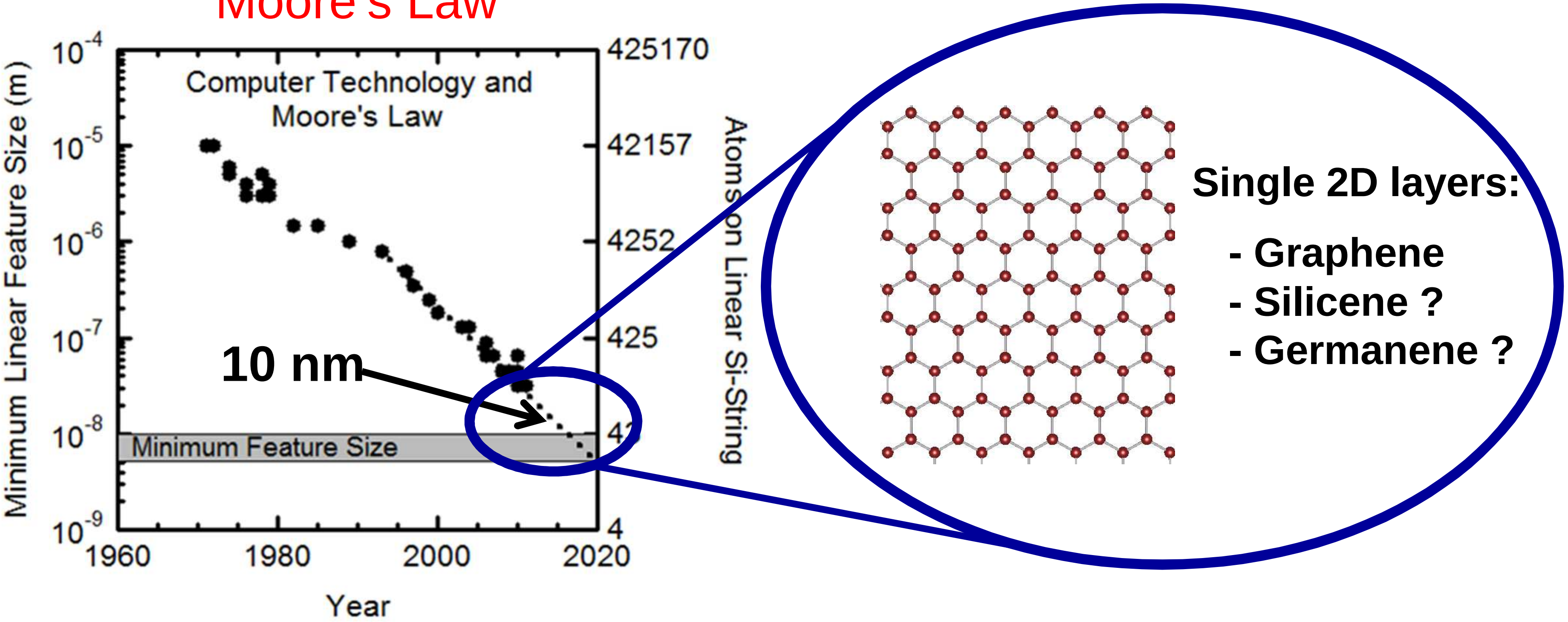
Carbon	→	**Graphene**
Silicon	→	**Silicene**
Germanium	→	**Germanene**

Introduction

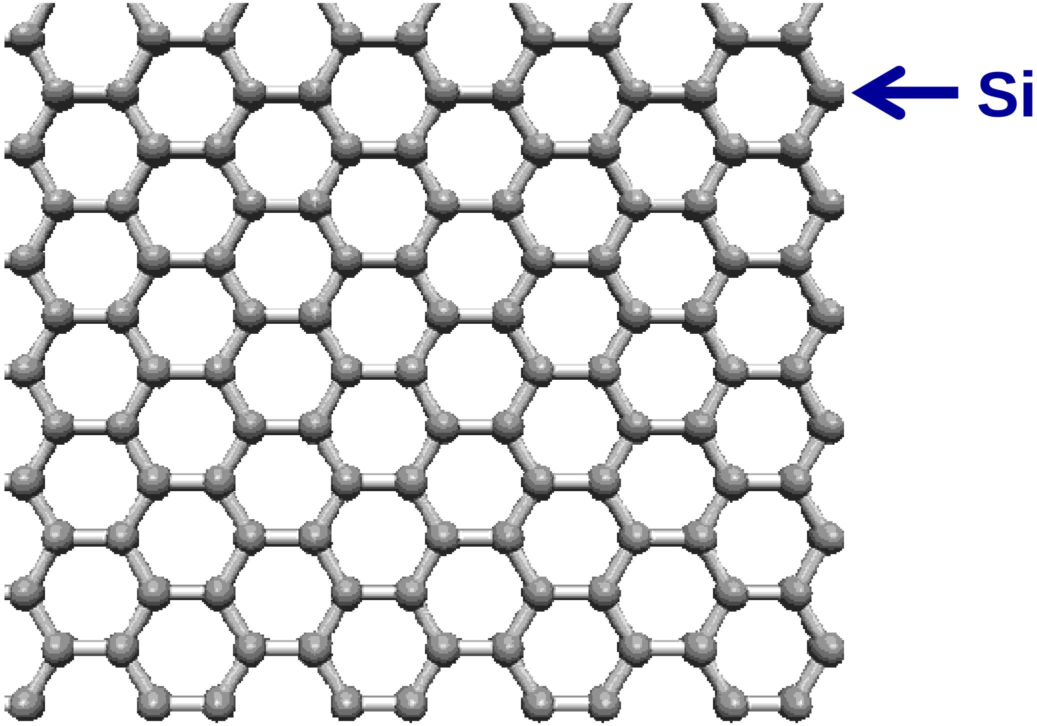


Moore's Law

Breaking the limit of Moore's Law



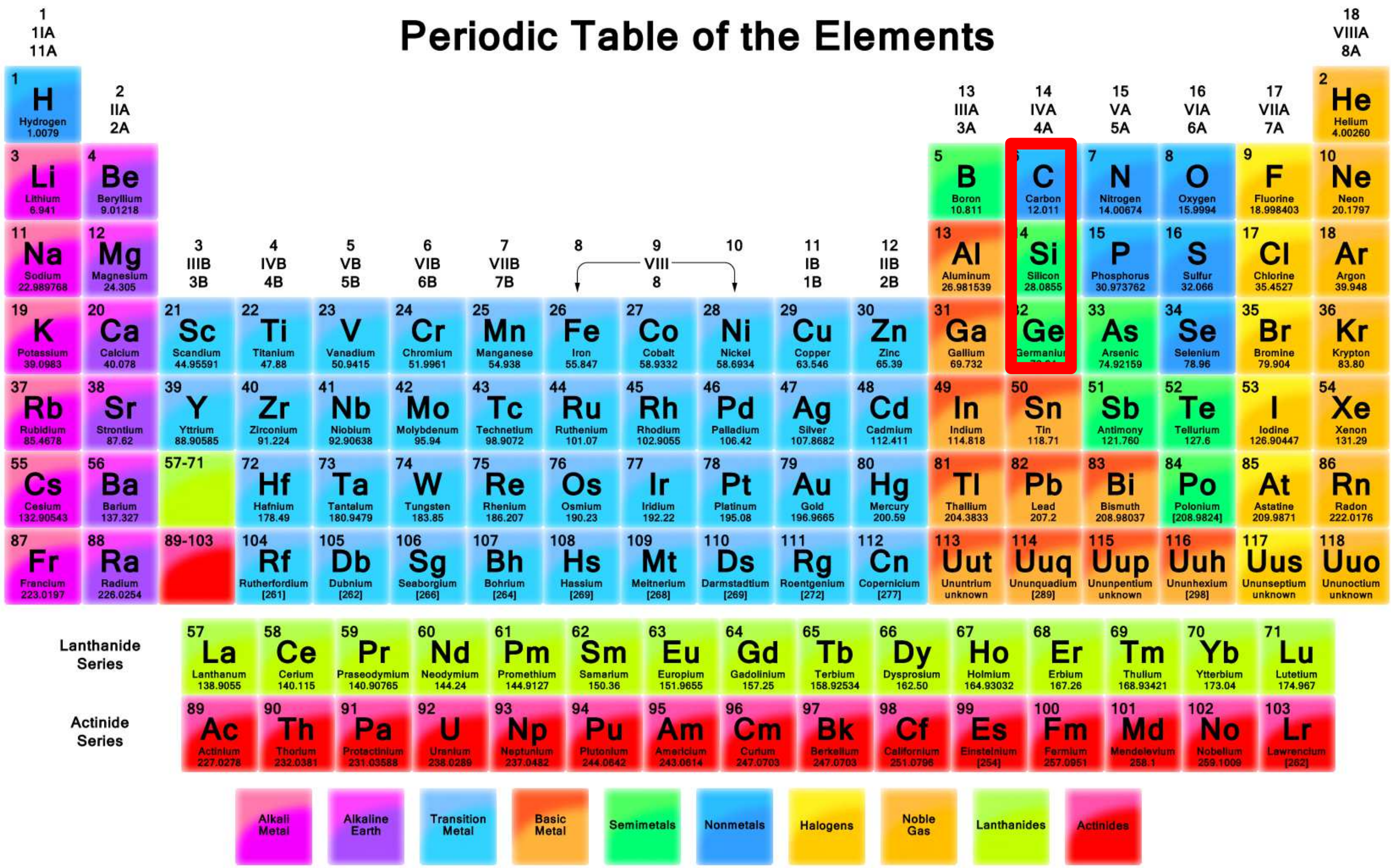
Silicene



Silicene Synthesis ? YES

Electronic properties ?

Introduction



Introduction

Electronic configuration

Carbon

[He] $2s^2\ 2p^2$

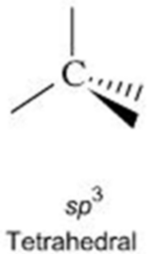
$E_{C_{2s}} = 19.4$ eV
$E_{C_{2p}} = 10.7$ eV

Silicon

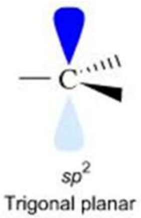
[Ne] $3s^2\ 3p^2$

$E_{Si_{3s}} = 15.0$eV
$E_{Si_{3p}} = 7.8$eV

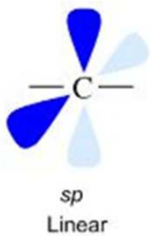
$$E_{C_{2s}} - E_{C_{2p}} = 8.7\text{eV} \quad > \quad E_{Si_{2s}} - E_{Si_{2p}} = 7.2 \text{ eV}$$



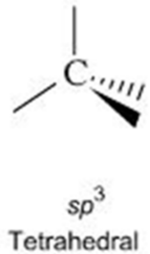
Diamond



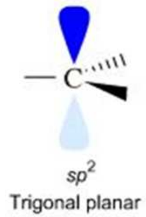
Graphite



Acetylene



Silicon (Diamond)



Silicene ???

Introduction

Electronic configuration

Carbon

[He] $2s^2$ $2p^2$

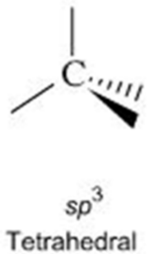
$E_{C_{2s}} = 19.4$ eV
$E_{C_{2p}} = 10.7$ eV

Germanium

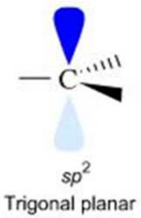
[Ar] $4s^2$ $4p^2$

$E_{Ge_{4s}} = 15.6$ eV
$E_{Ge_{4p}} = 7.5$ eV

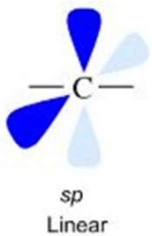
$E_{C_{2s}} - E_{C_{2p}} = 8.7$eV $>$ $E_{Ge_{4s}} - E_{Ge_{4p}} = 8.1$ eV



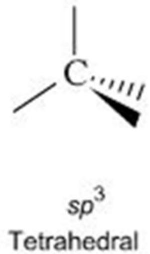
Diamond



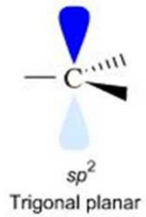
Graphite



Acetylene

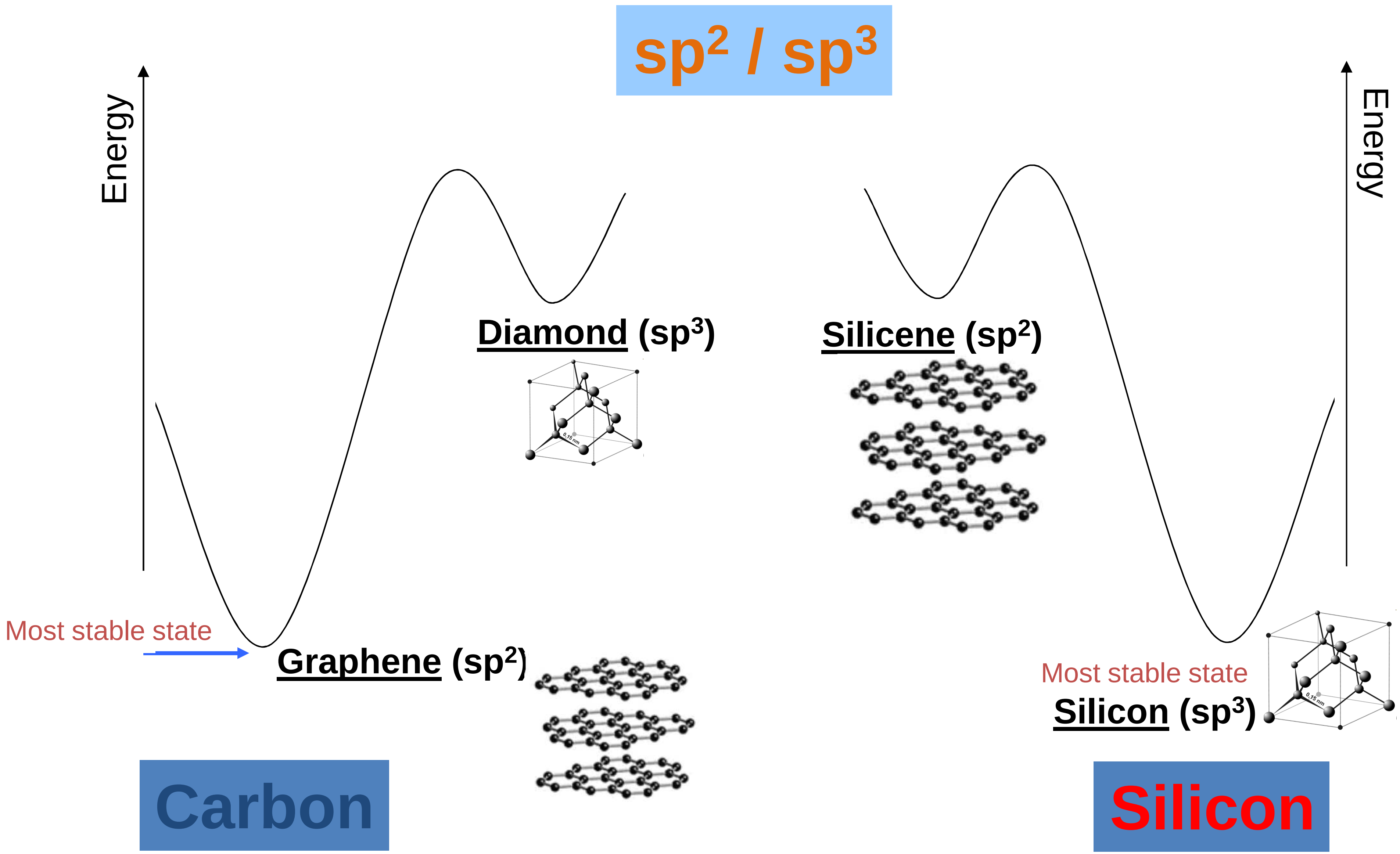


Germanium (Diamond)

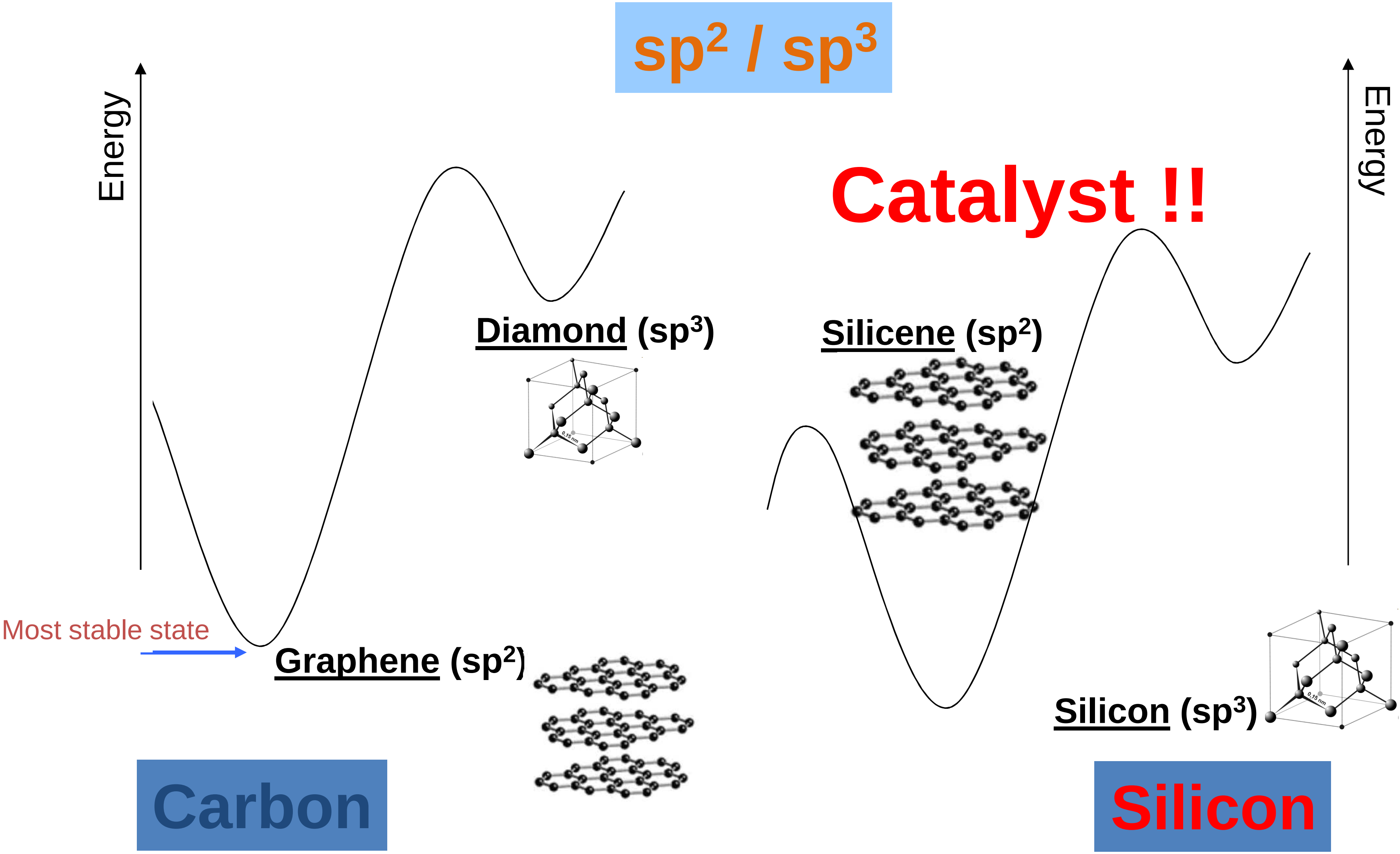


Germanene???

Introduction

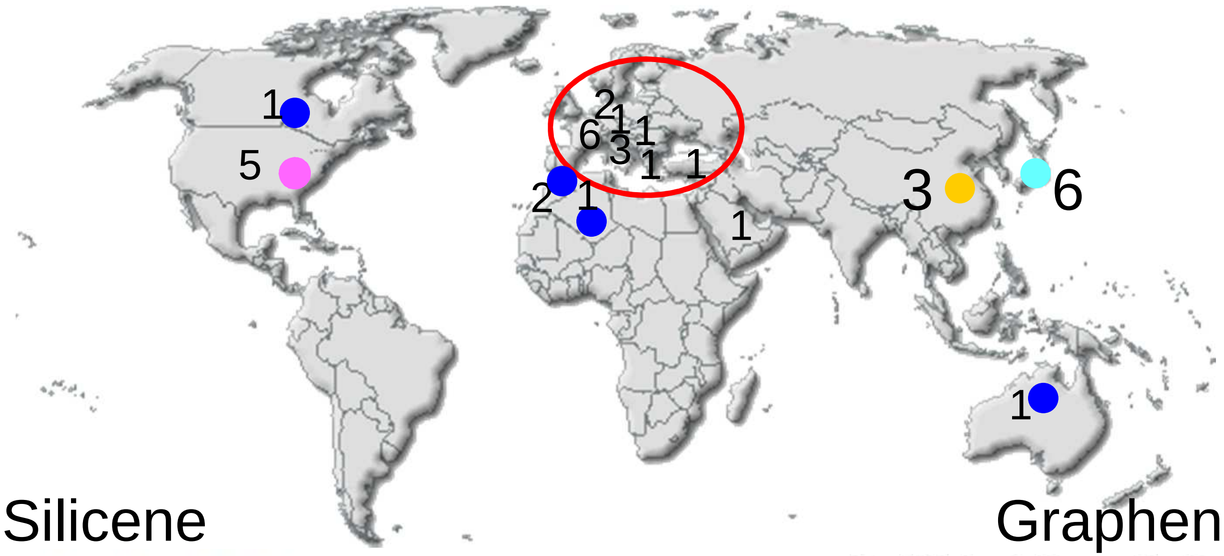


Introduction

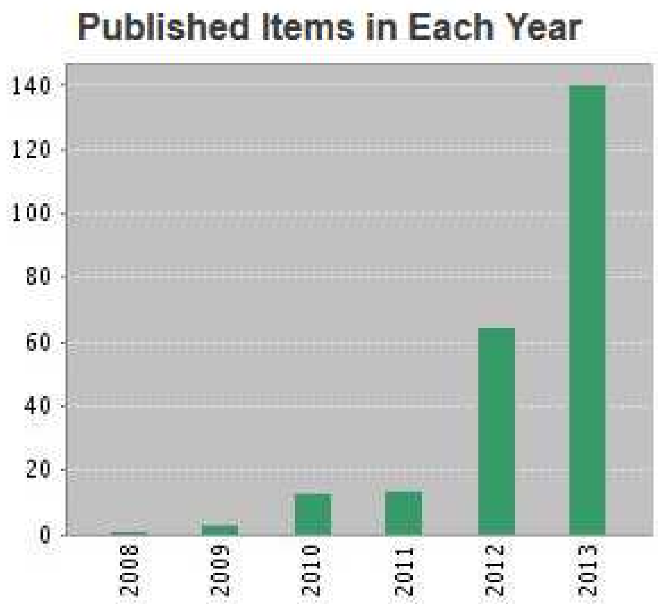


Silicene across the World

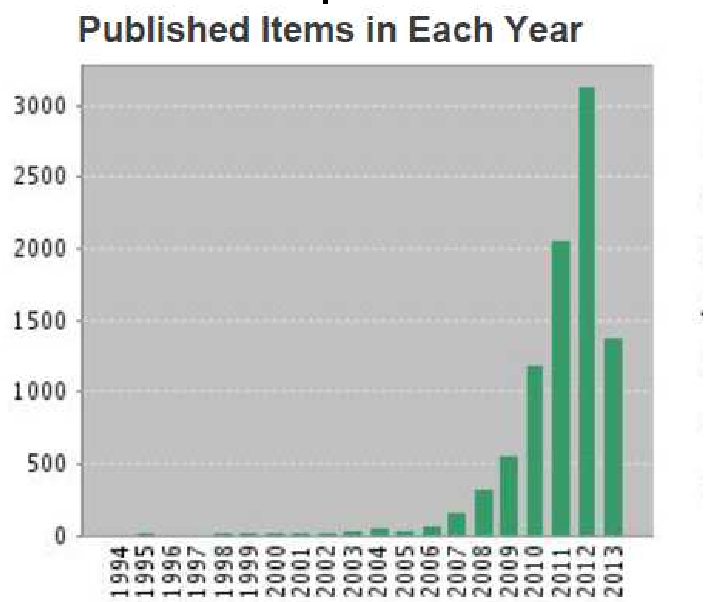
Worldewide contributions



Silicene



Graphene



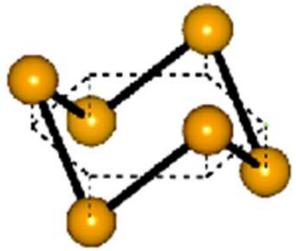
Quick history

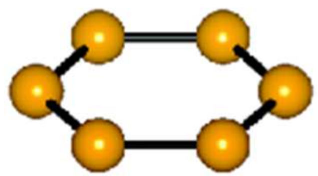
Theoretical study

Stability and electronic properties :

(TB) G. Guzmán-Verri, et al, Phys. Rev. B 76, 075131 (2007)
(DFT) S. Lebègue et al, Phys. Rev. B 79 115409 (2009)
(DFT) Cahangirov et al, Phys. Rev. Let. 102, 236804, (2009)

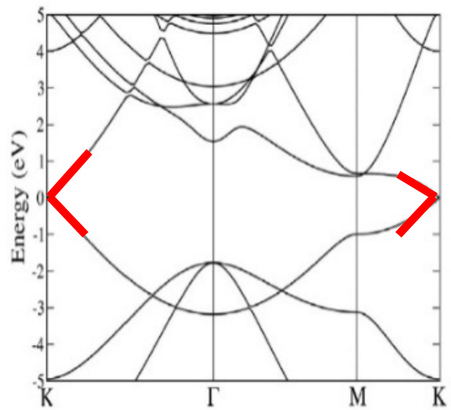
Silicene **Graphene**





- Silicene is a buckled layer

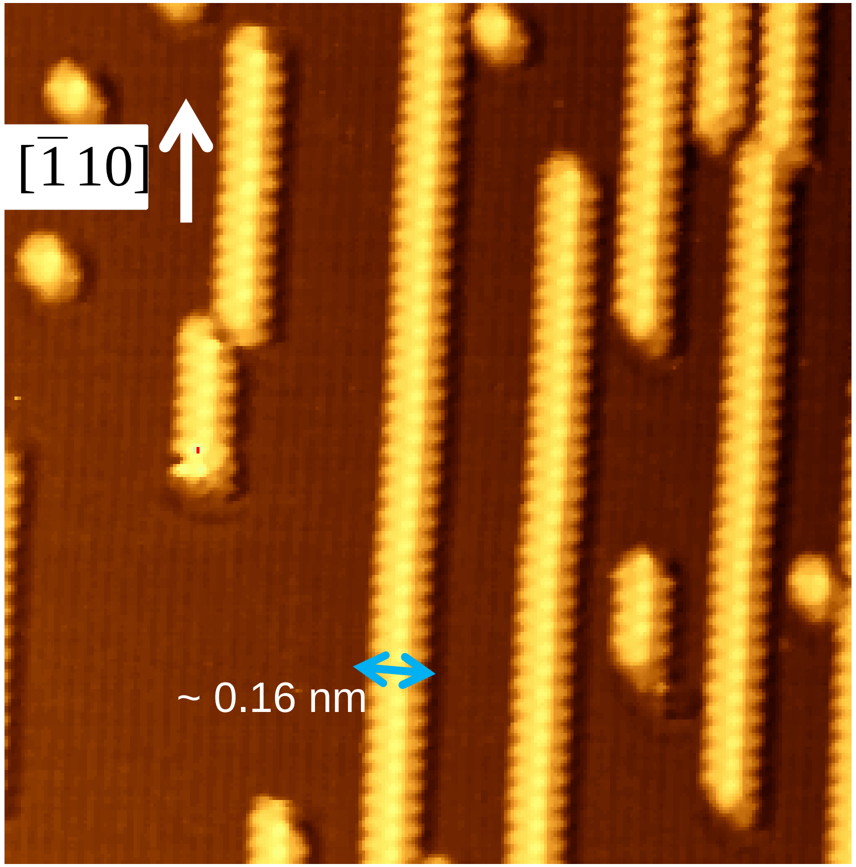
- Silicene has intrinsic stability and an electronic structure similar to the one of graphene.



S. Lebègue et al, Phys. Rev. B 79 115409 (2009)

Si/Ag(110) at RT

Ordered Si Nanoribbons with the same width (0.16 nm)



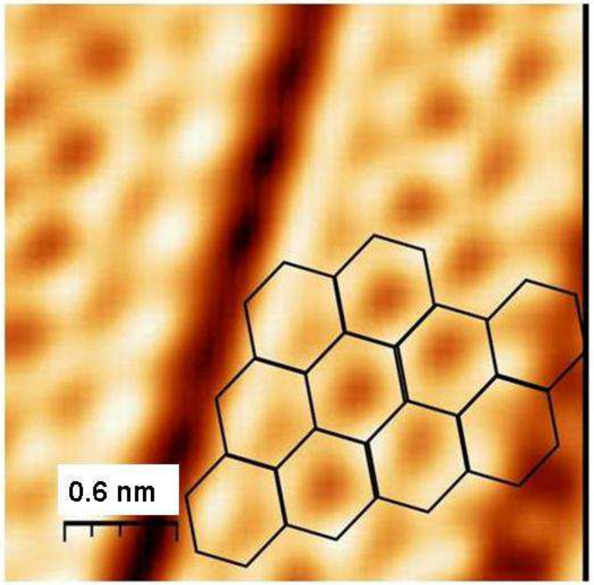
22x22 nm^2

Léandri et al. Surf. Sci., 574, L9 (2005)

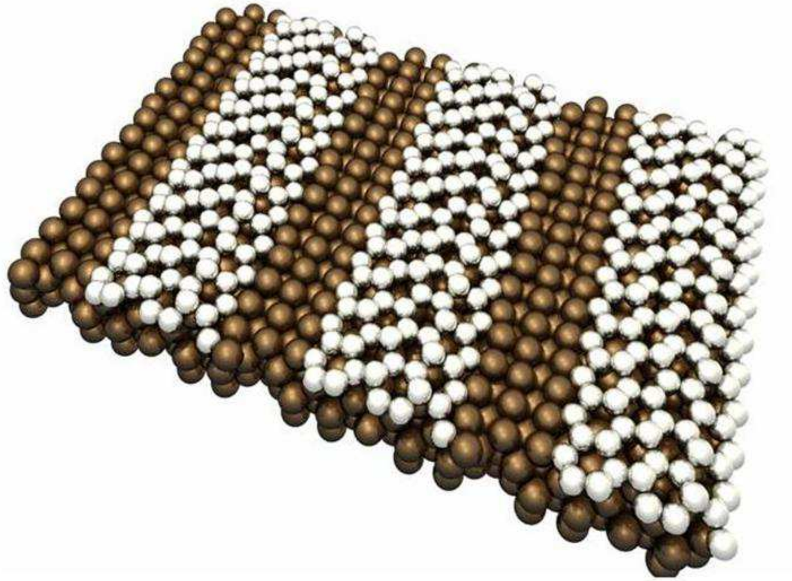
Silicene NRs

Si/Ag(110)

STM

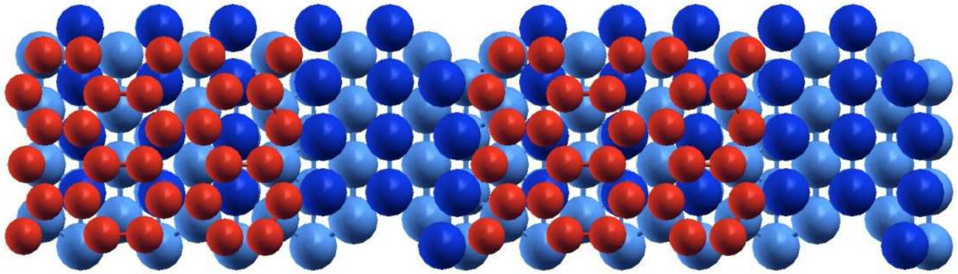


calculations



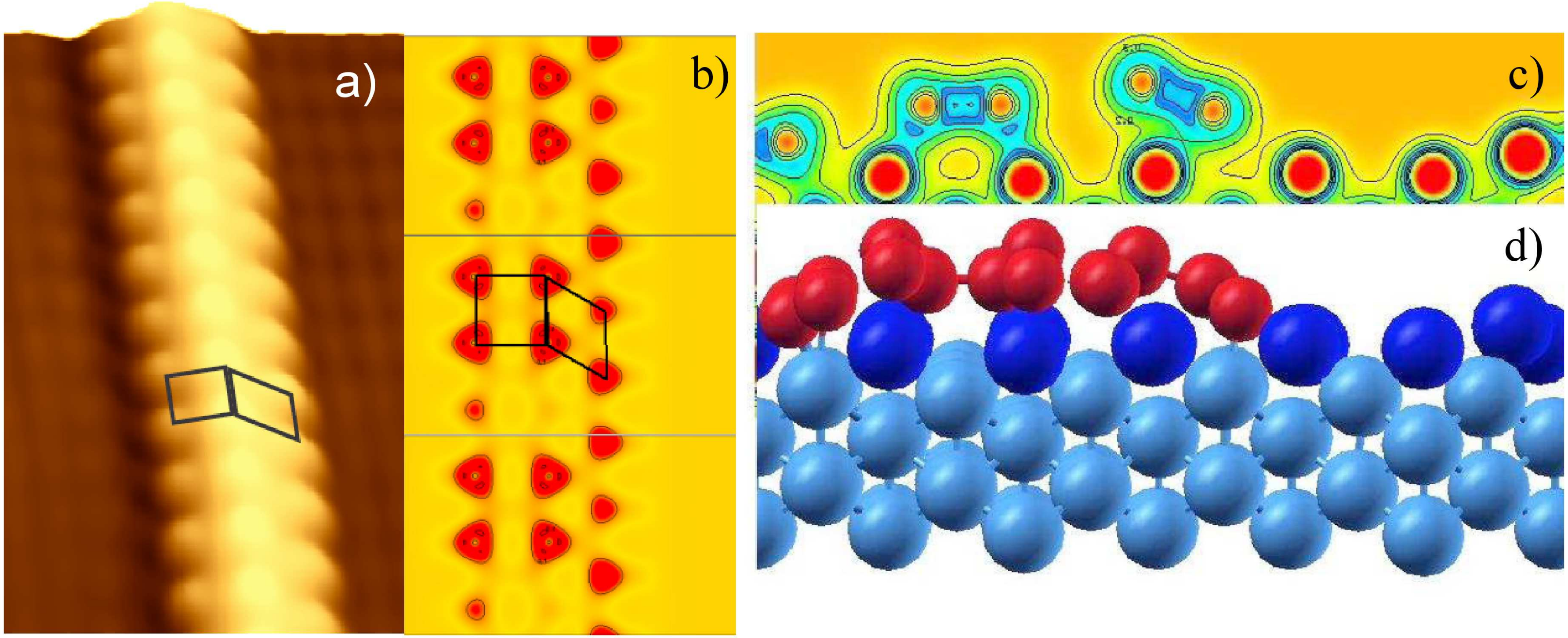
B. Aufray et al. Appl. Phys. Lett. 96, 183102 (2010)
A. Kara et al. Surf. Sci. Reports, 67, 1–18 (2012)

Silicene NRs on Ag(110) : Growth at RT



STM

Ab initio calculations

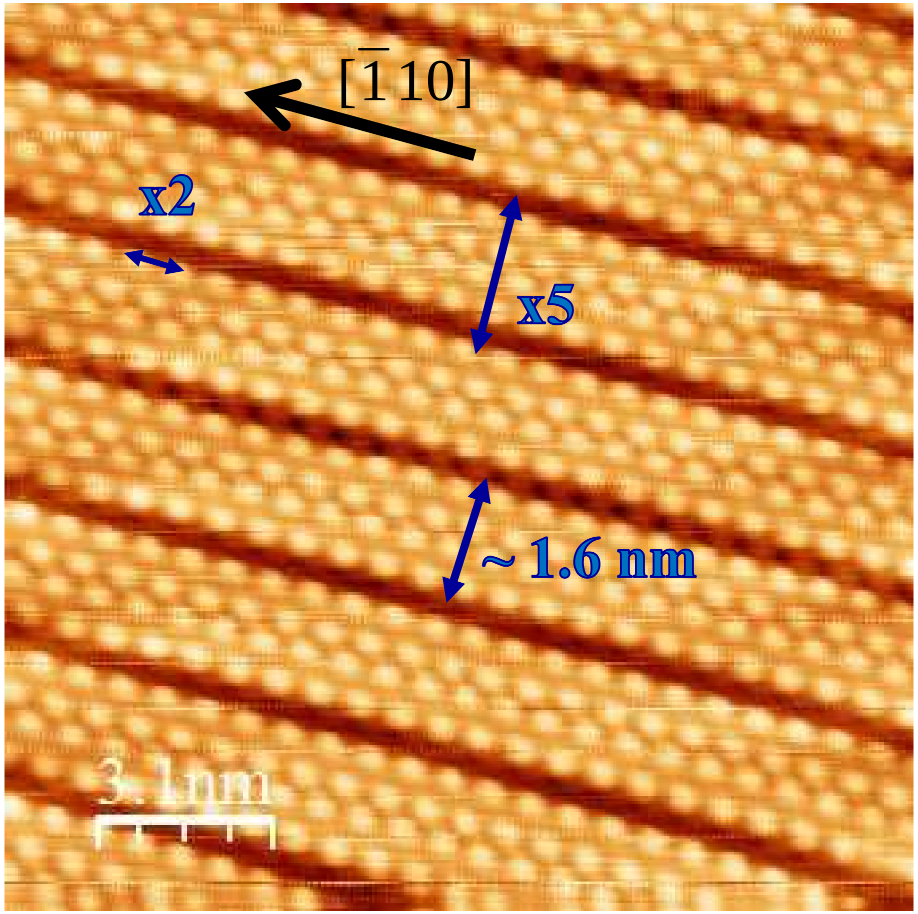


A. Kara et al. J. Phys. Condens. Matter 22, 045004 (2010)

Silicene NRs on Ag(110) : Growth at 220°C

<u>Deposition at 220°C:</u> 1 ML of Si/Ag(110)

STM



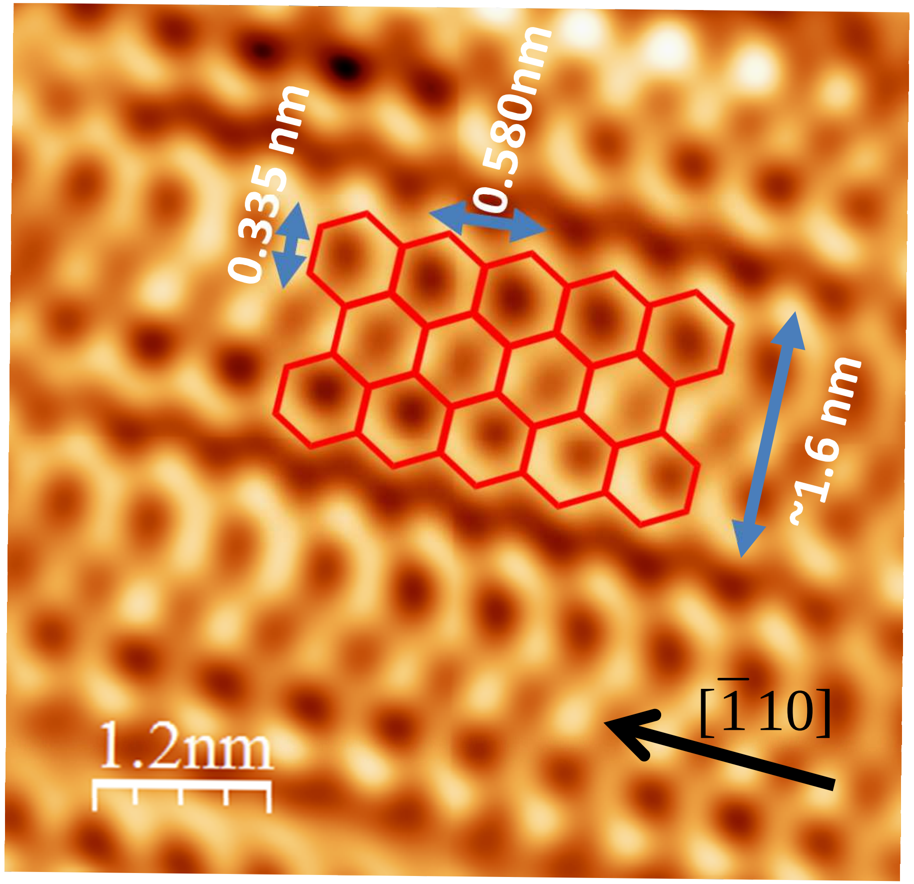
2x5 superstructure

15x15 nm^2 , V = -0.9 V ; I = 0.5 nA

Silicene NRs on Ag(110) : Growth at 220°C

<u>Deposition at 220°C:</u> 1 ML of Si/Ag(110)

STM

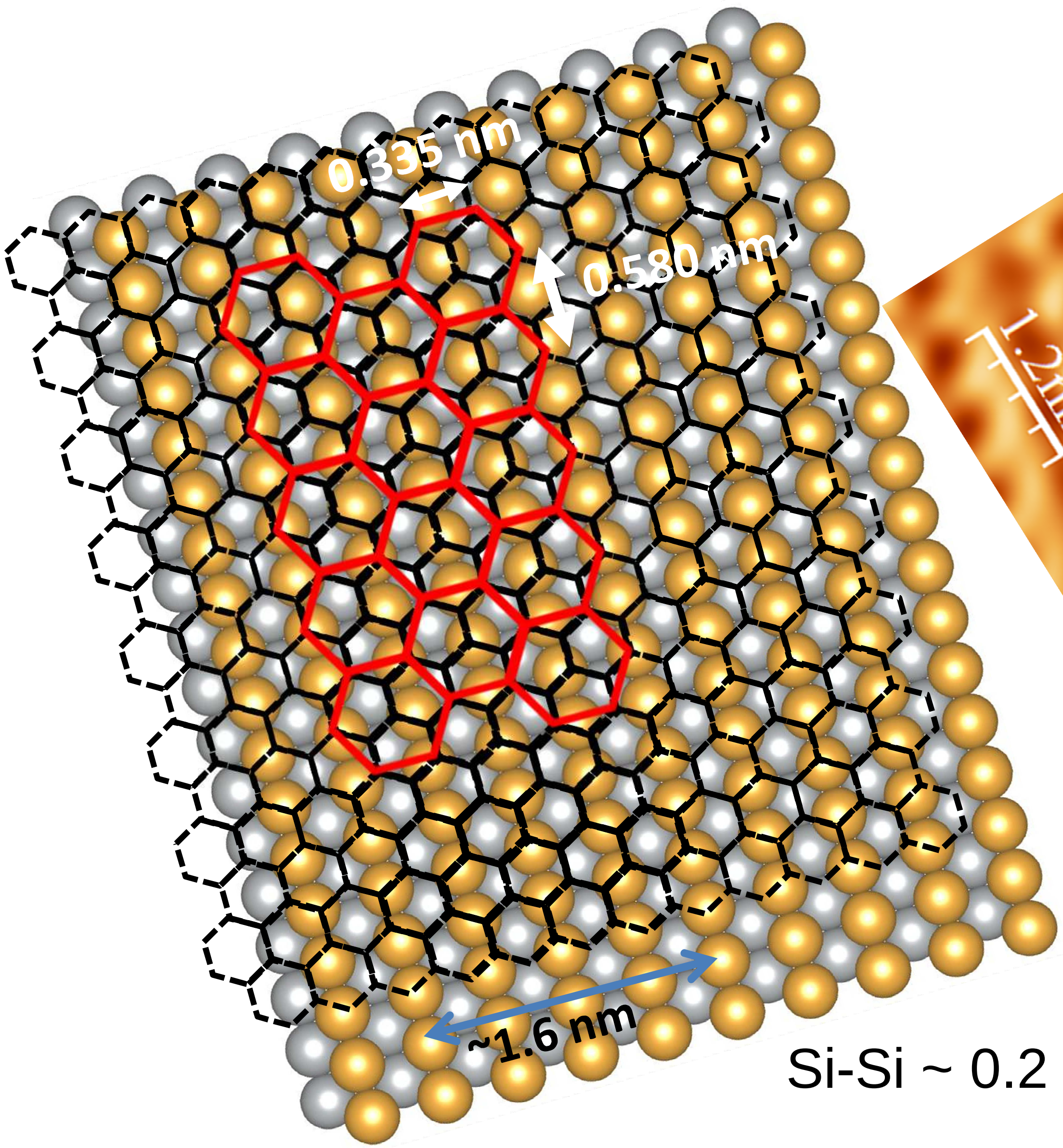


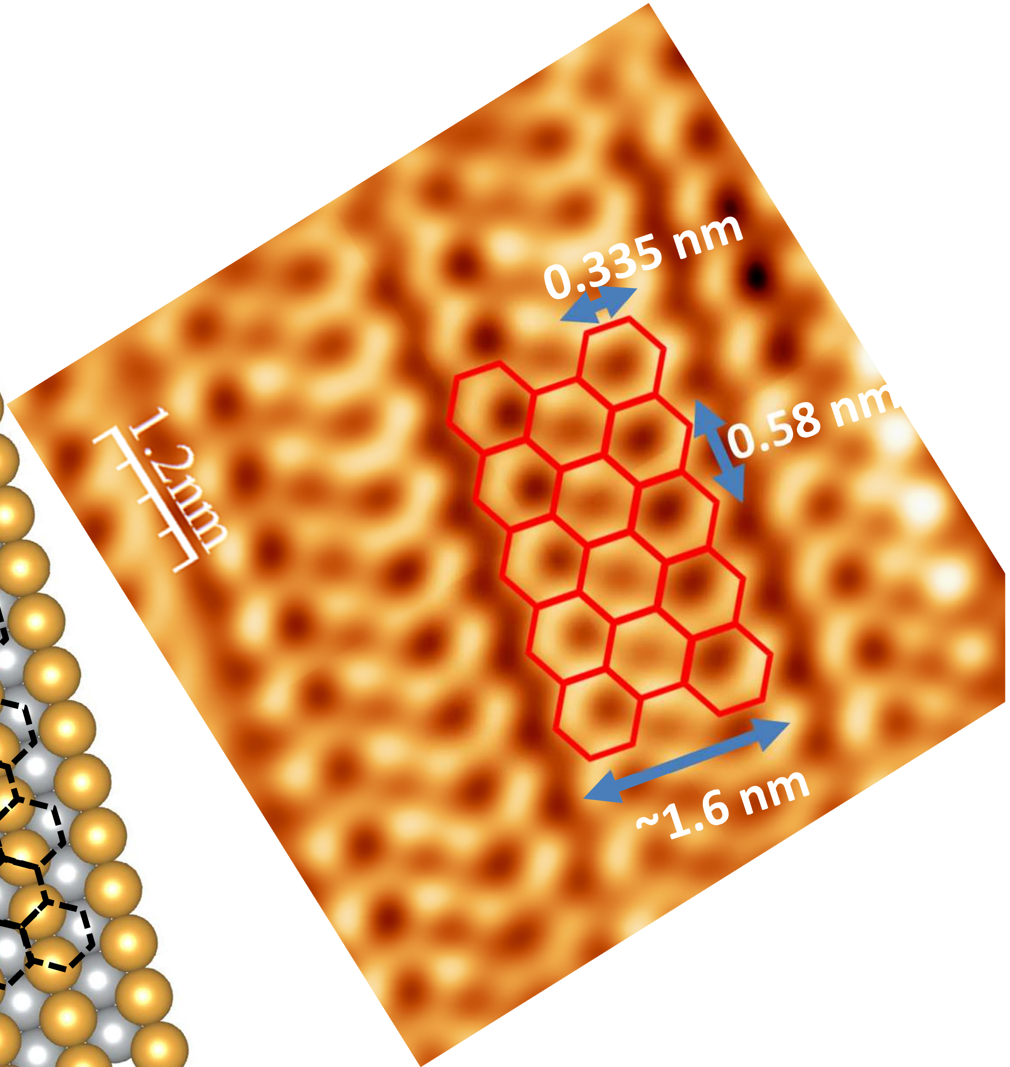
8x8 nm^2 , V = -1.6 V ; I = 3.2 nA

Self-assembled Si NRs

M. R. TCHALALA et al. (accepted)

Silicene NRs on Ag(110) : Growth at 220°C





Si-Si ~ 0.2 nm

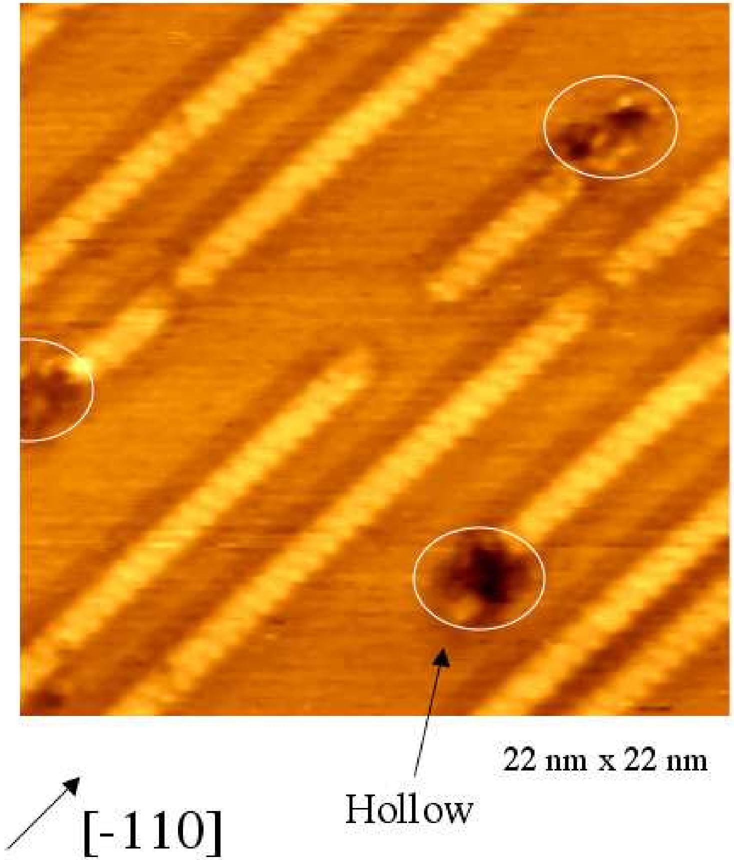
M. R. TCHALALA et al. (accepted)

Isloted Silicene NRs: molecular oxidation

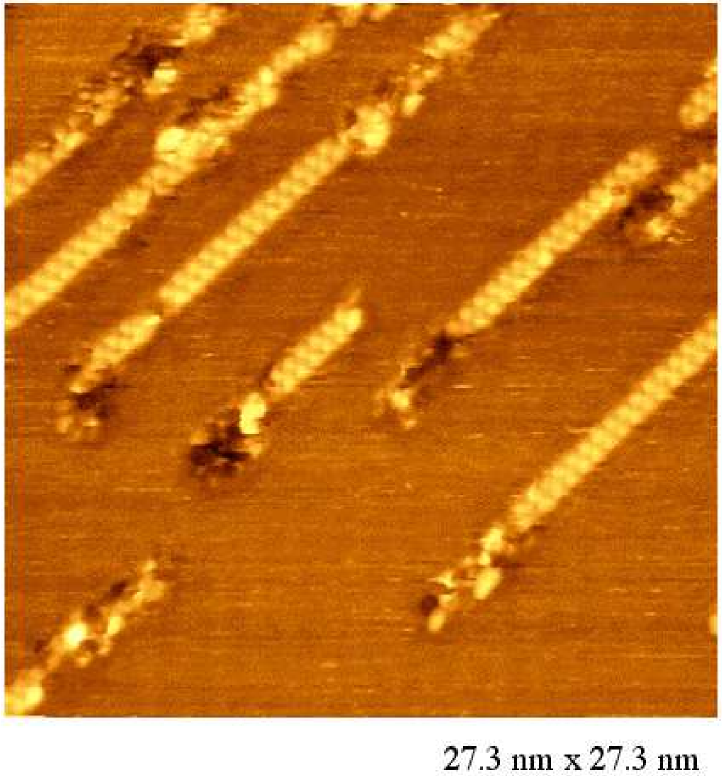
Chemical reactivity toward O_2

STM

15 L



30 L



Oxidation starts from the NRs extremities

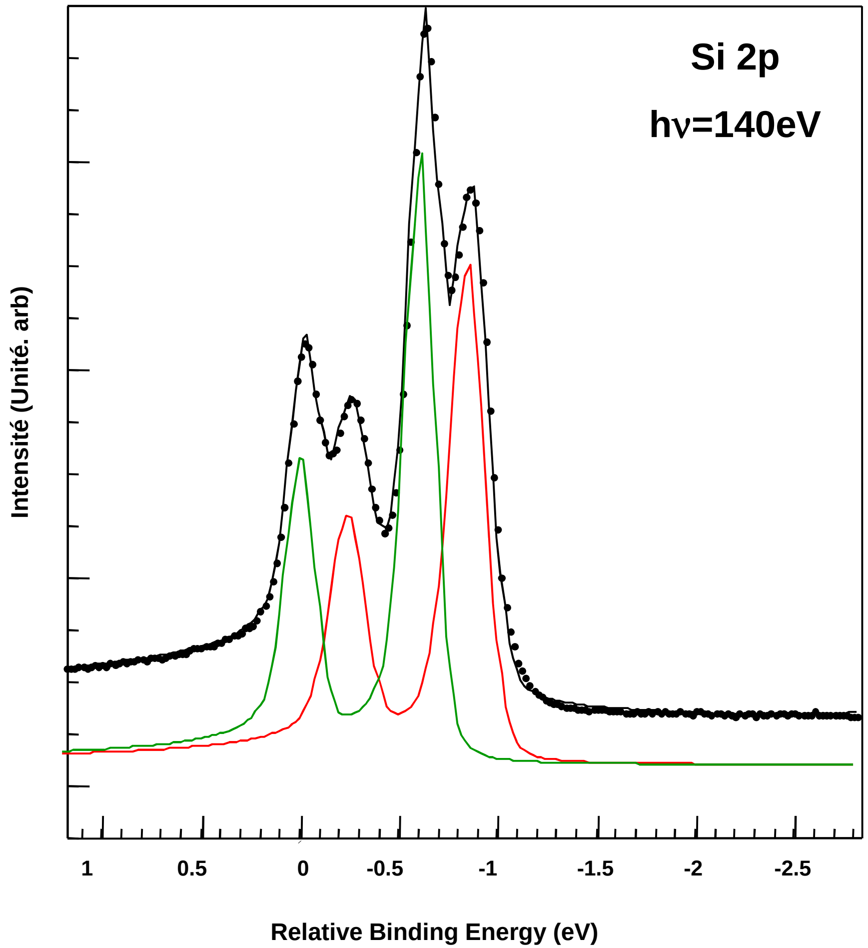
De. Padova et al. Nano Letters 8 (8), 2299-2304 (2008)

Silicene NRs on Ag(110)

Core Level Photo-Electron Spectroscopy (Synchrotron radiation)

PES

θ ≈ 0,5 ML



Two components :

two well-defined Si environments:

Narrowest Si 2p core-levels

Atomically perfect Si nano-ribbons!

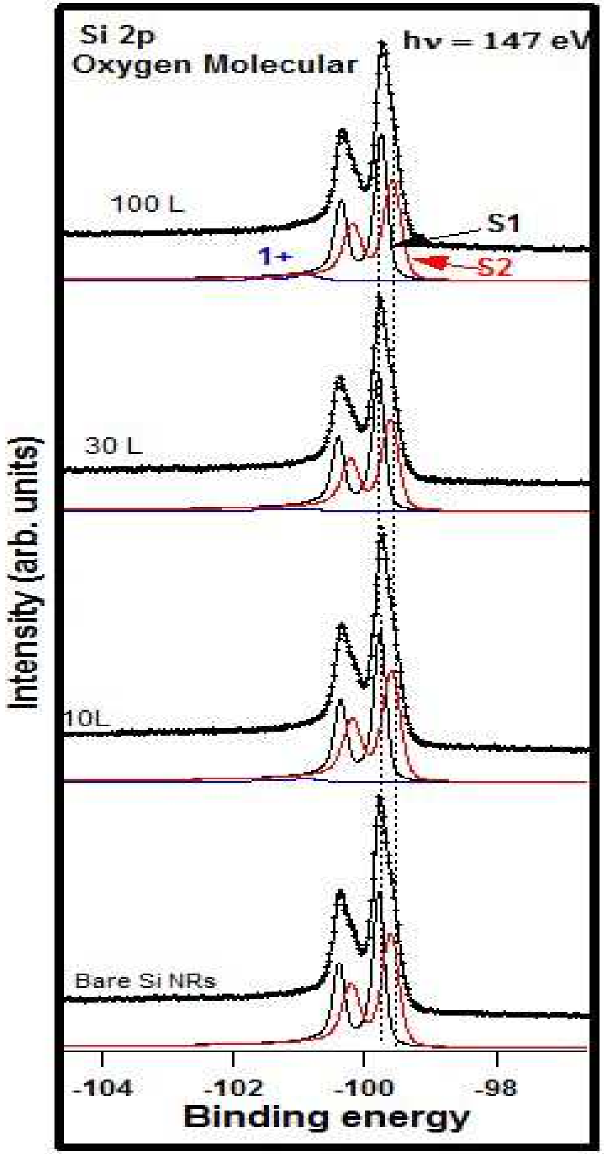
asymmetry : 0.12

Metallic character

C. Leandri *et al*. Surf. Sci., **574**, (2005) L9
De Padova *et al*., Nano Letters **8** (2008) 271
De. Padova et al. Appl. Phys. letters, 96, 261905 (2010)

Assembled silicene NRs: molecular oxidation

Core Level Photo-Electron Spectroscopy (Synchrotron radiation) PES

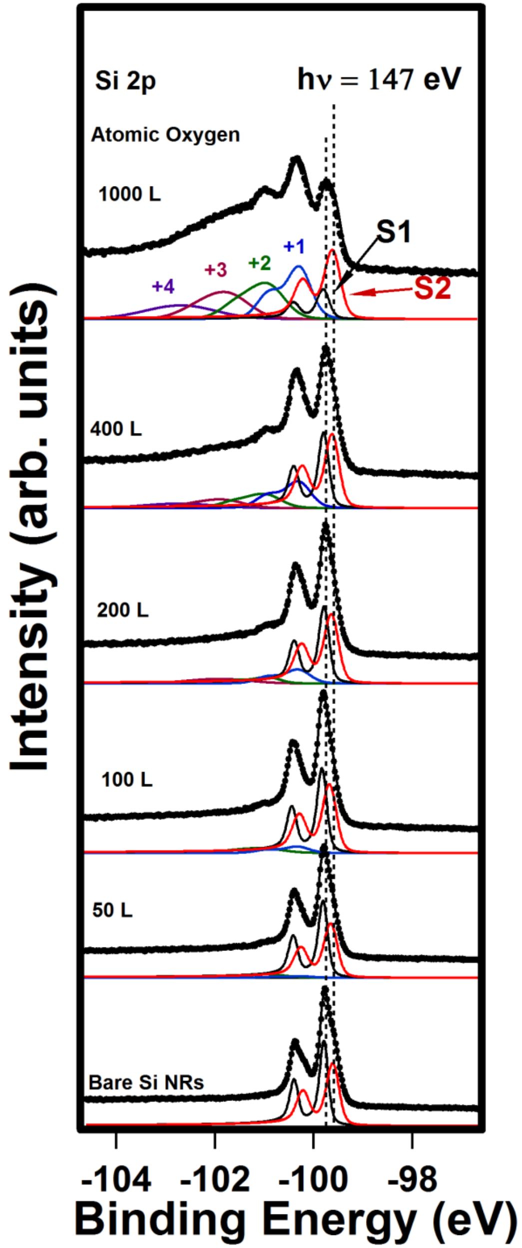


Silicene NRs are not reactive to molecular Oxygen

Assembled silicene NRs: Atomic oxidation

Core Level Photo-Electron Spectroscopy (Synchrotron radiation)

PES



Silicene NRs are more reactive to atomic Oxygen

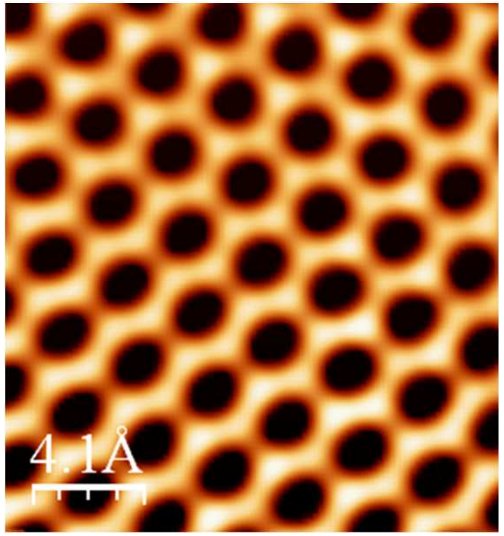
Reactivity toward oxygen

Graphene **Silicene** **Silicon (Sp^3)**

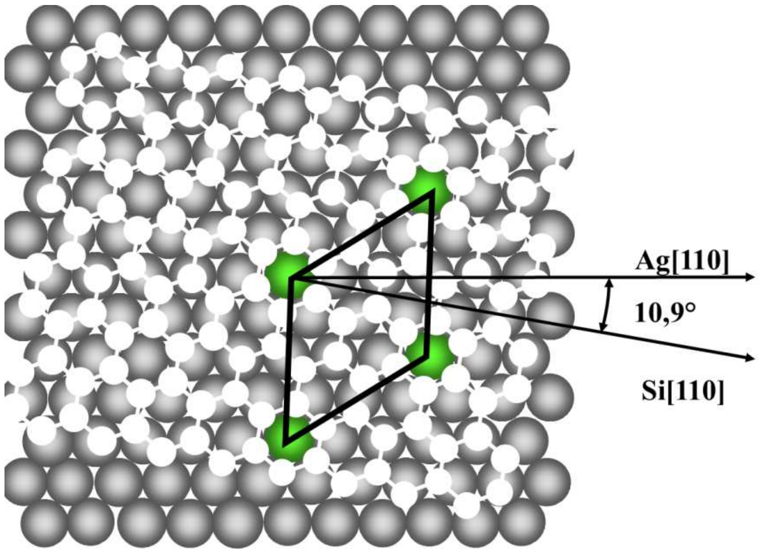
Silicene sheet

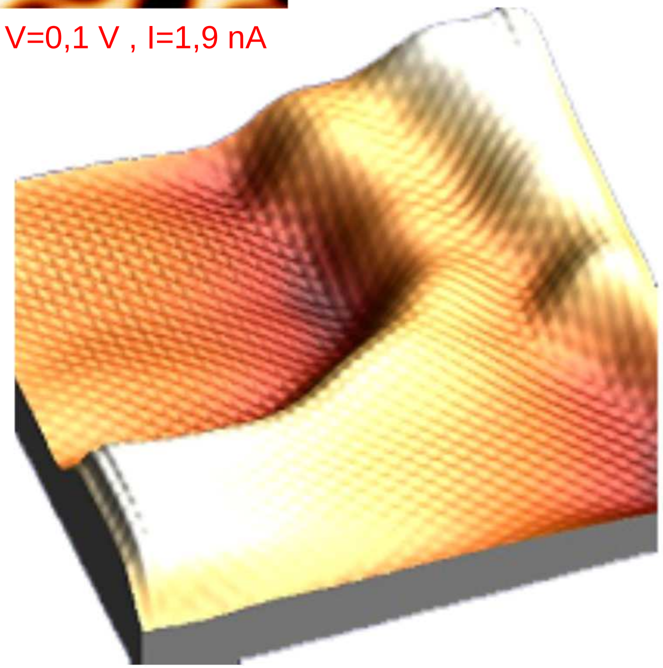
Si/Ag(111)

(2√3 x 2√3)R30°



22x22 nm^2 , V=0,1 V , I=1,9 nA





B. Lalmi etal, APL, 97, 223109 (2010)

Silicene sheet

Si/Ag(111)

STM

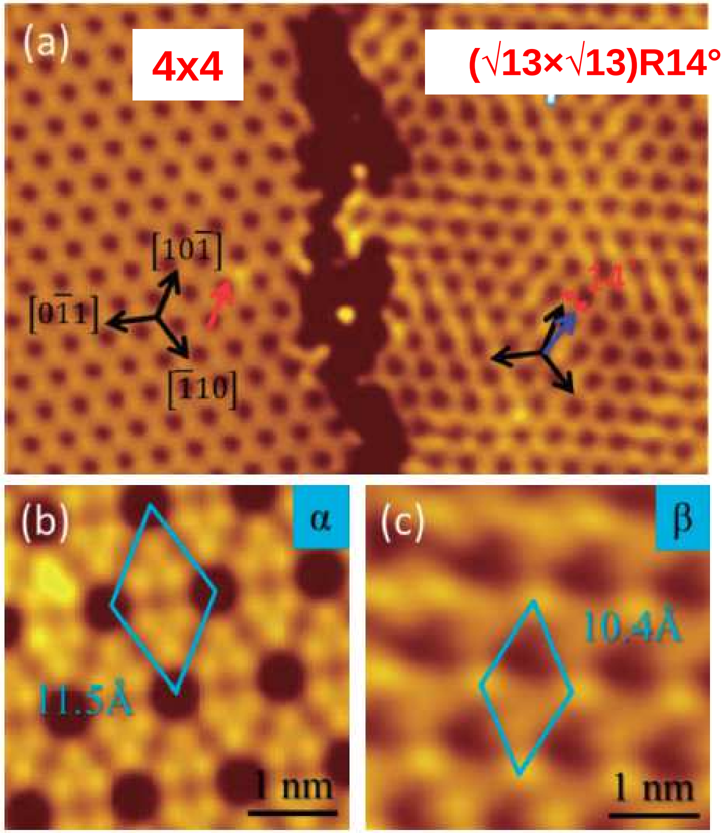


Fig. 1. (a) Topographic STM image (22.7 × 15.1 nm^2) of silicene on Ag(111) taken at 6 K with the tunneling current (I) of 0.2 nA and sample bias (V) of −0.7 V. The red and blue arrows show the direction of a unit vector of α and β structures, respectively. The black arrows show three highly symmetric axes of Ag(111). Highly resolved topographic images of (b) α ($I = 0.2$ nA, $V = 0.5$ V) and (c) β ($I = 0.3$ nA, $V = -0.02$ V) phases taken at 6 K. Both image sizes are 3.8 × 3.8 nm^2.

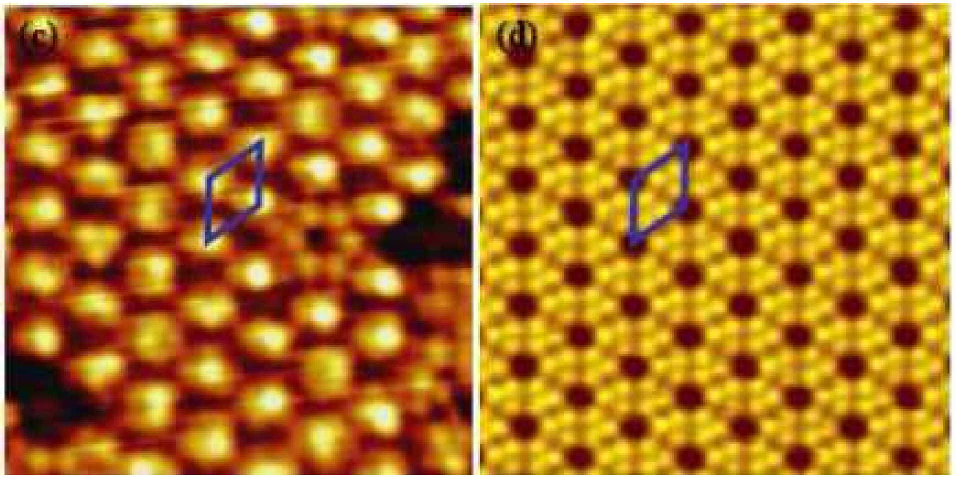
Chun-Liang Lin et al . Applied Physics Express 5 (2012)

Silicene sheet

Si/Ag(111)

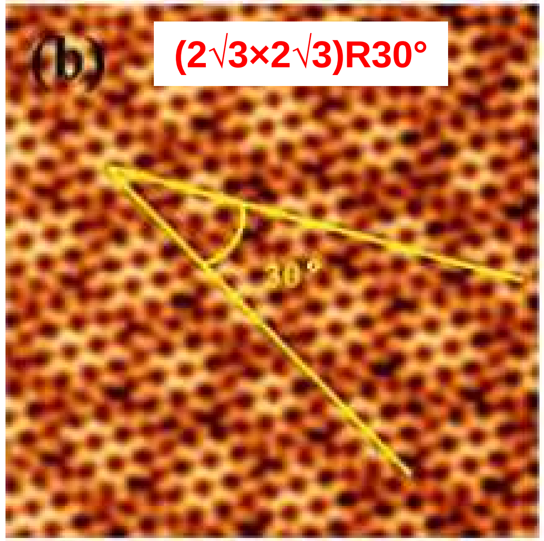
4x4

STM



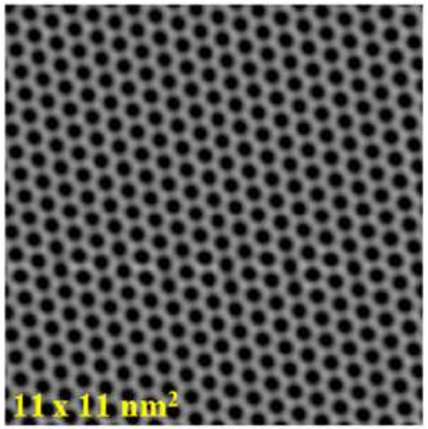
420 K　　460 K

480 K

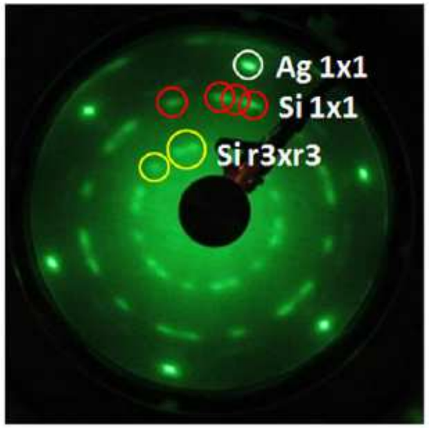


single layer of silicene

(a)



(b)

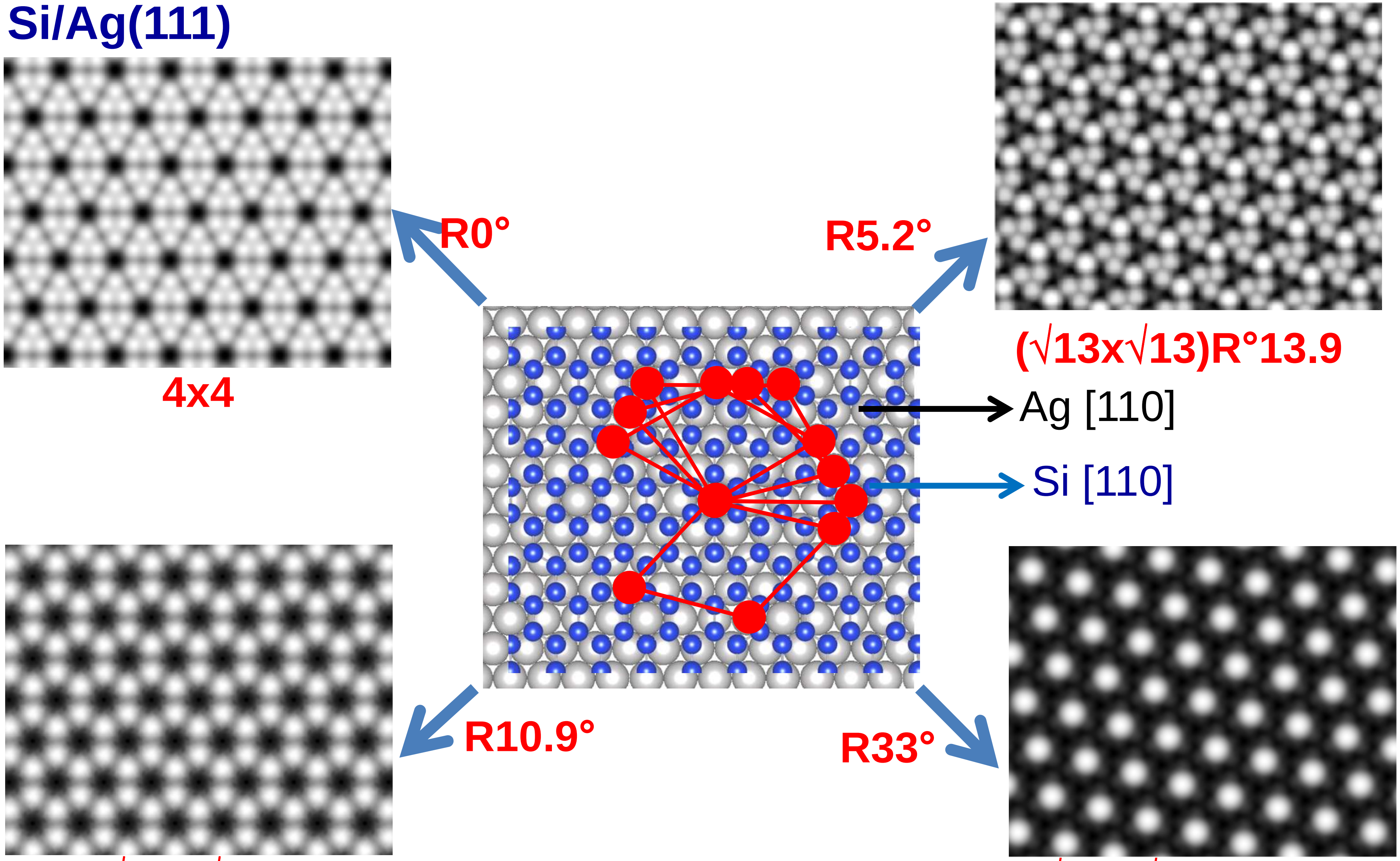


(√3×√3)R30°

Lan Chen et al, Phys. Rev. Lett., 110, 085504 (2013)
Baojie Feng et al, Nano Lett., 12 (7), 3507 (2012)

Silicene sheet

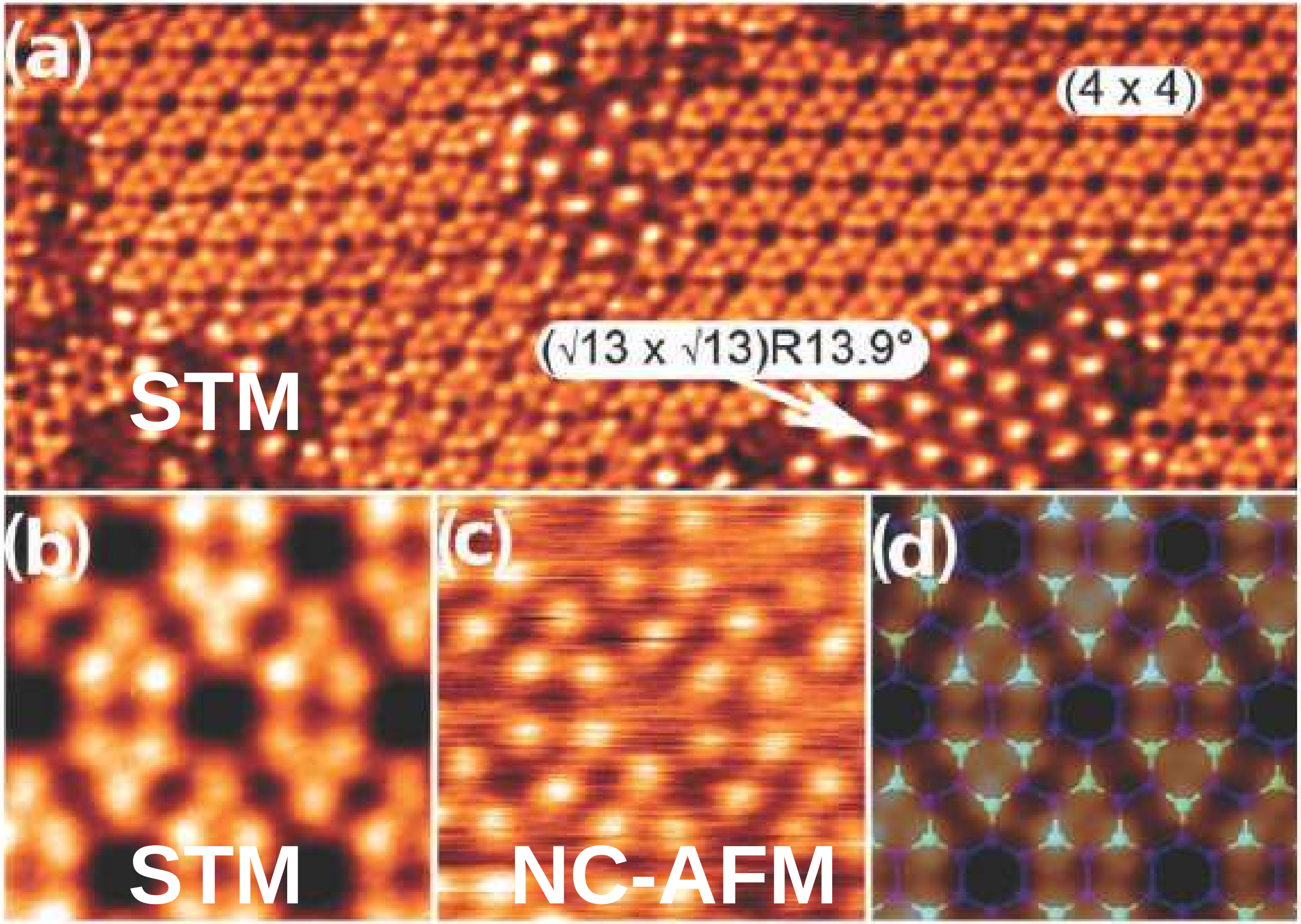
Si/Ag(111)



H. Enriquez *et al.* Journal. of Phys. Condens. Matter, 24, 314211 (2012)

Silicene sheet

Si/Ag(111) : STM and nc-AFM



Z. Majzik J. Phys.: Condens. Matter, 25, 225301 (2013)

Silicene NRs

Si/ZrB2 (0001)

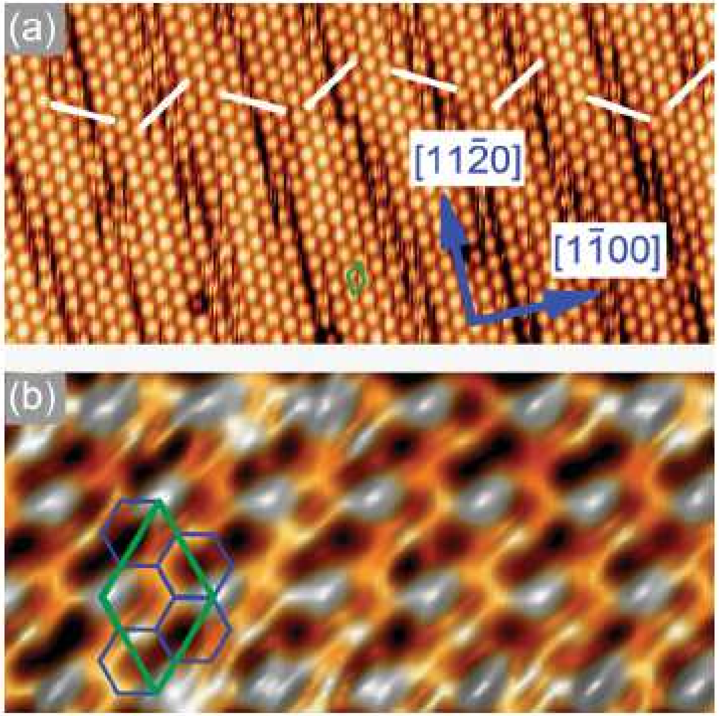
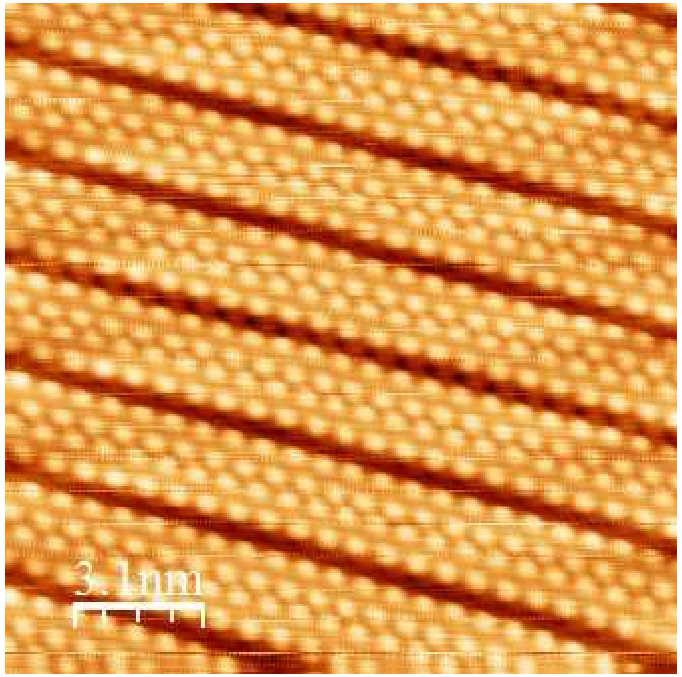


FIG. 1 (color). STM images of the (2×2)-reconstructed $ZrB_2(0001)$ surface with different length scales: (a) 20 nm$\times$ 9.5 nm, $I = 55$ pA, $V_s = 700$ mV, (b) 4.2 nm $\times$ 2 nm, $I =$ 600 pA, $V_s = 100$ mV. The white lines emphasize the direction of offsets between successive domains. The (2×2) UC and the honeycomb mesh are emphasized by green and blue solid lines, respectively.



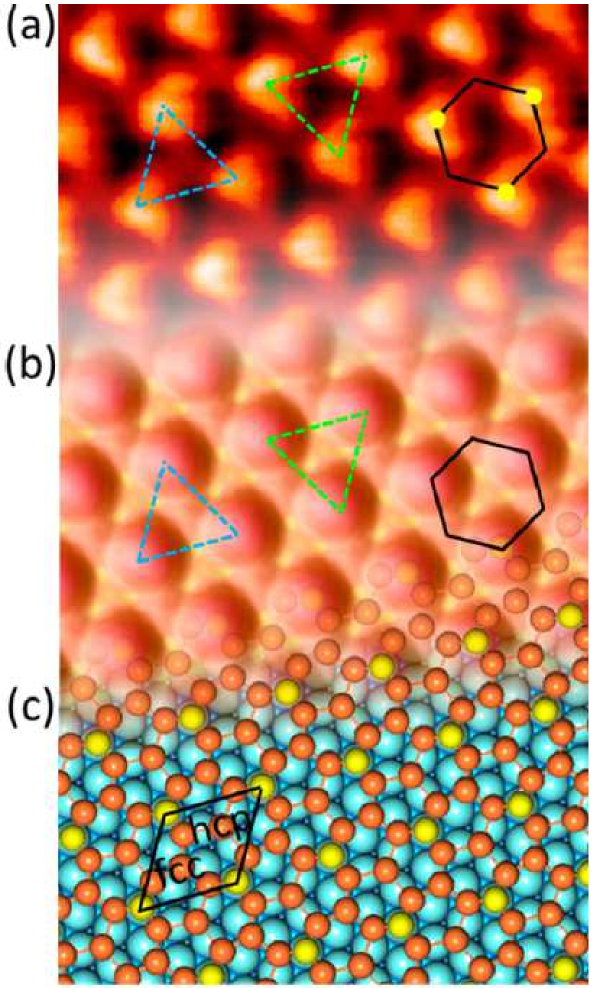
15x15 nm^2 , V = -0.9 V ; I = 0.5 nA

Silicene on Ag(110)

A. Fleurence etal. PRL 108, 245501 (2012)

Silicene sheet

Si/Ir(111)



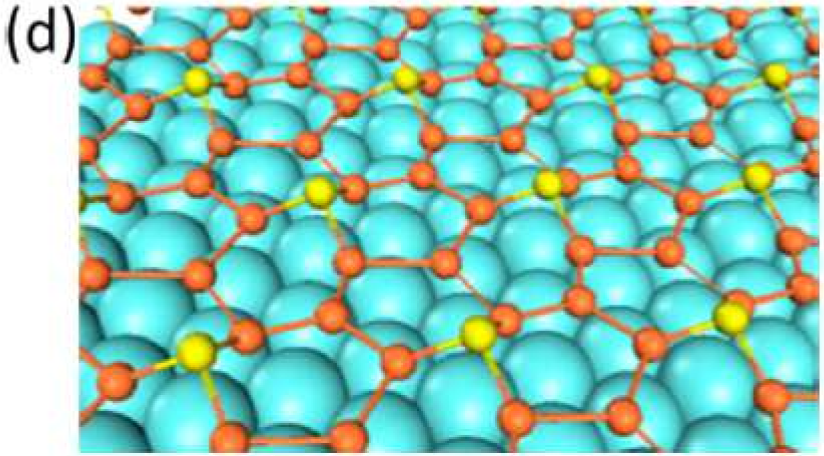
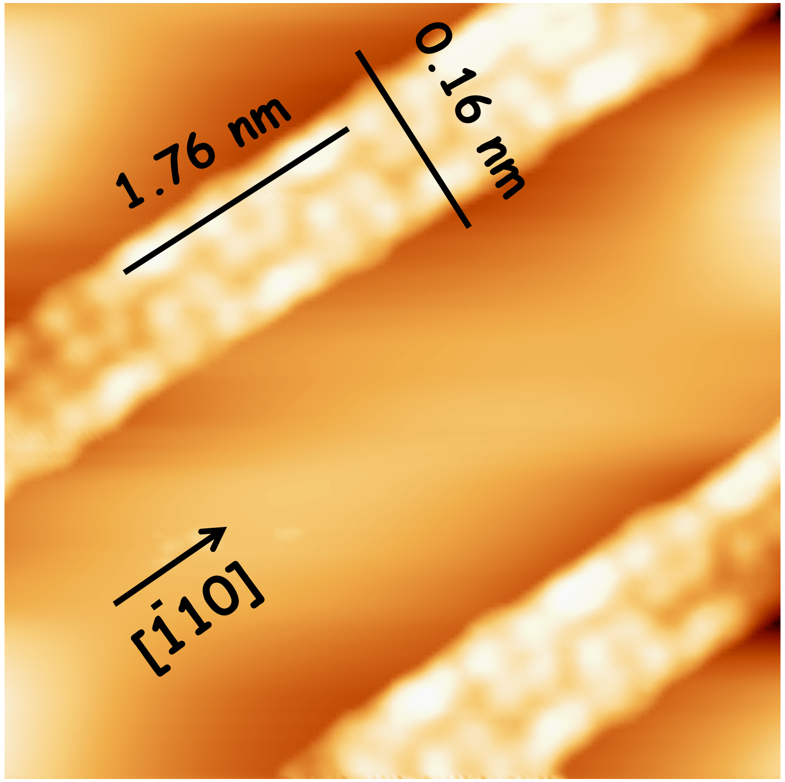
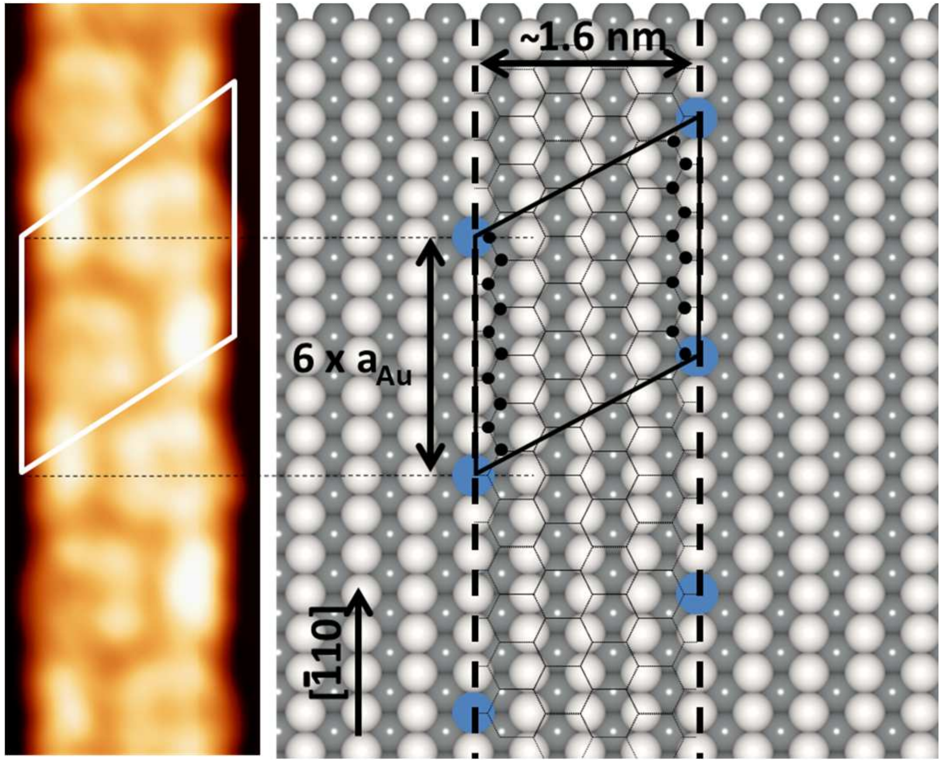


Figure 3. (a) Zoomed-in STM image of the silicon layer. Besides the brightest protrusions, two other regions showing different contrast are indicated by the upward and downward triangles. The honeycomb feature is indicated by the black hexagon. (b) Simulated STM image, showing features identical with the experimental results in the same triangles and hexagons. (c) Top view of the relaxed atomic model of the $(\sqrt{3}\times\sqrt{3})$silicene/$(\sqrt{7}\times\sqrt{7})$Ir(111) configuration. (d) Perspective view of the relaxed model in c, showing an undulated silicene on Ir(111) surface.

Lei Meng et al. Nano Lett., 2013, 13 (2), pp 685–690

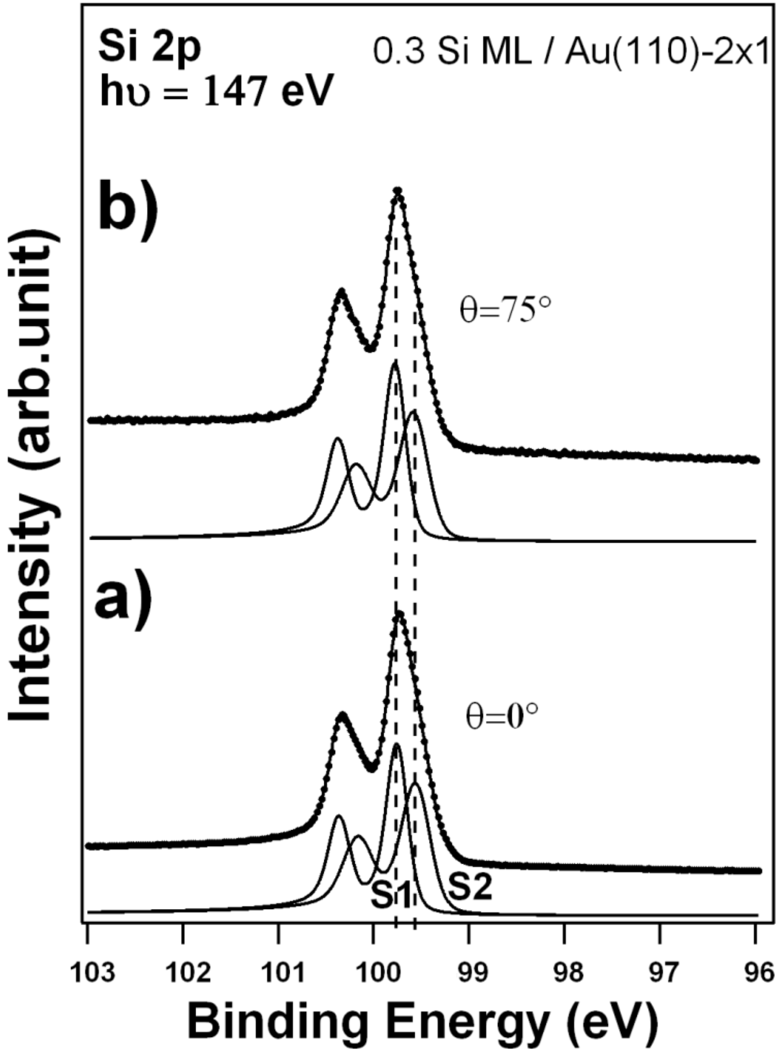
Si/Au(110)





M. R. TCHALALA et al. APL, 102, 083107 (2013)

Si NRs on Au(110)-2x1



S1 → Silicon within the NRs

S2 → Silicon at the NRS edges

Two well defined components

Asymmetry : 0.09

↓

Two Si environments

M. R. TCHALALA et al. APL, 102, 083107 (2013)

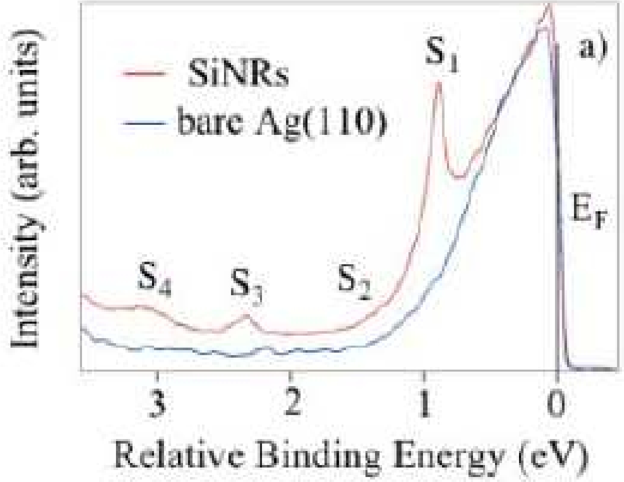
Silicene sheet:

Electronic properties

Dirac cone or no Dirac cone

Silicene NRs

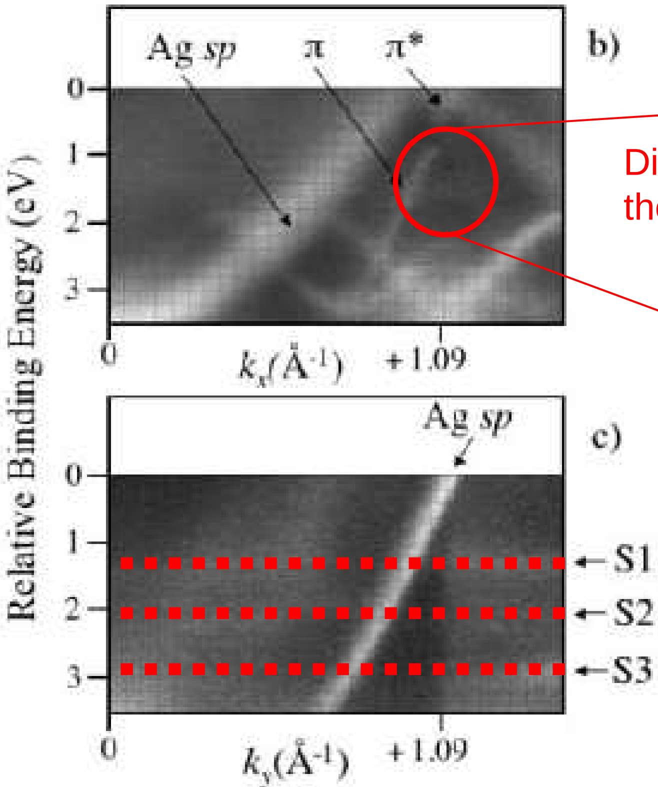
Si/Ag(110)



New electronic states

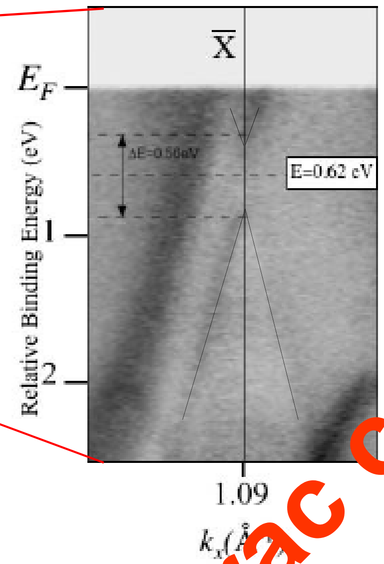
➡ **Quantum Confinement**

The silicon band dispersion along the direction of the nano-ribbons shows the Dirac cone like graphene



Dispersion along the nanoribbons

Dispersion perpendicular to the nanoribbons



Dirac cone

De. Padova et al. Appl. Phys. letters, 96, 261905 (2010)

Silicene sheet:

Si/Ag(111)

Electronic properties (HRPES)

(4x4) superstructure

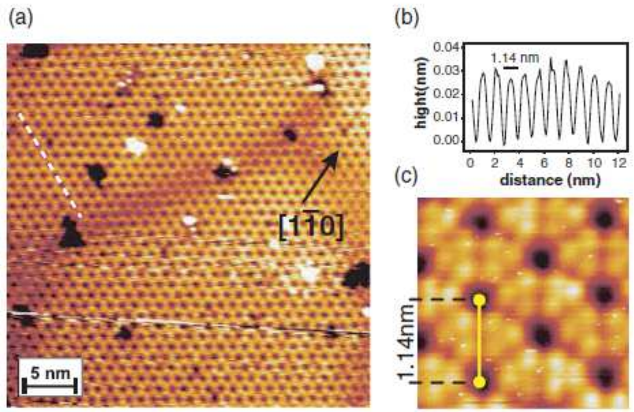


FIG. 2 (color). (a) Filled-states STM image of the 2D Si layer on Ag(111)-(1 × 1) ($U_{bias} = -1.3$ V, $I = 0.35$ nA). Clearly visible is the honeycomblike structure. (b) Line profile along the dashed white line indicated in (a). The dark centers in the STM micrograph are separated by 1.14 nm, corresponding to 4 times the Ag(111) lattice constant, in agreement with the (4 × 4) symmetry. (c) High-resolution STM topograph (3 × 3 nm, $U_{bias} = -1.3$ V, $I = 0.35$ nA) of the Si adlayer.

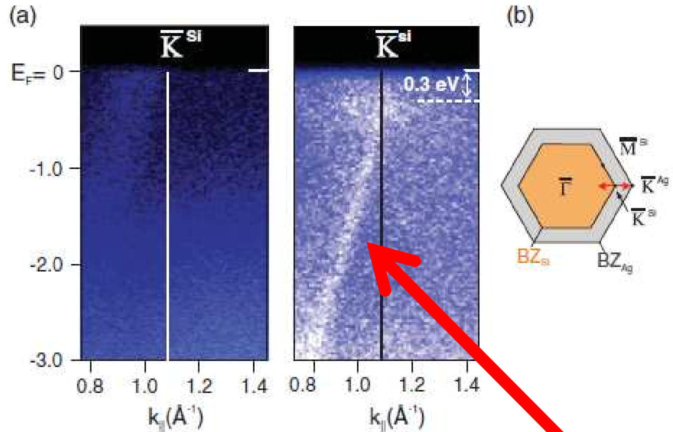


FIG. 3 (color). (a) ARPES intensity map for the clean Ag surface (left) and after formation of the 2D Si layer (right), taken along the Ag $\bar{\Gamma}$-$\bar{K}$ direction through the silicene $\bar{K}$($h\nu$ = 126 eV). (b) Brillouin-zone (BZ) scheme of the 2D Si layer with respect to the Ag(111)-(1 × 1) surface. The red arrow indicates the ARPES measurement direction.

Dirac cone

Linear dispesion

P. Vogt et al. PRL 108, 155501 (2012)

Silicene sheet:

Si/Ag(111)

Electronic properties (STS)

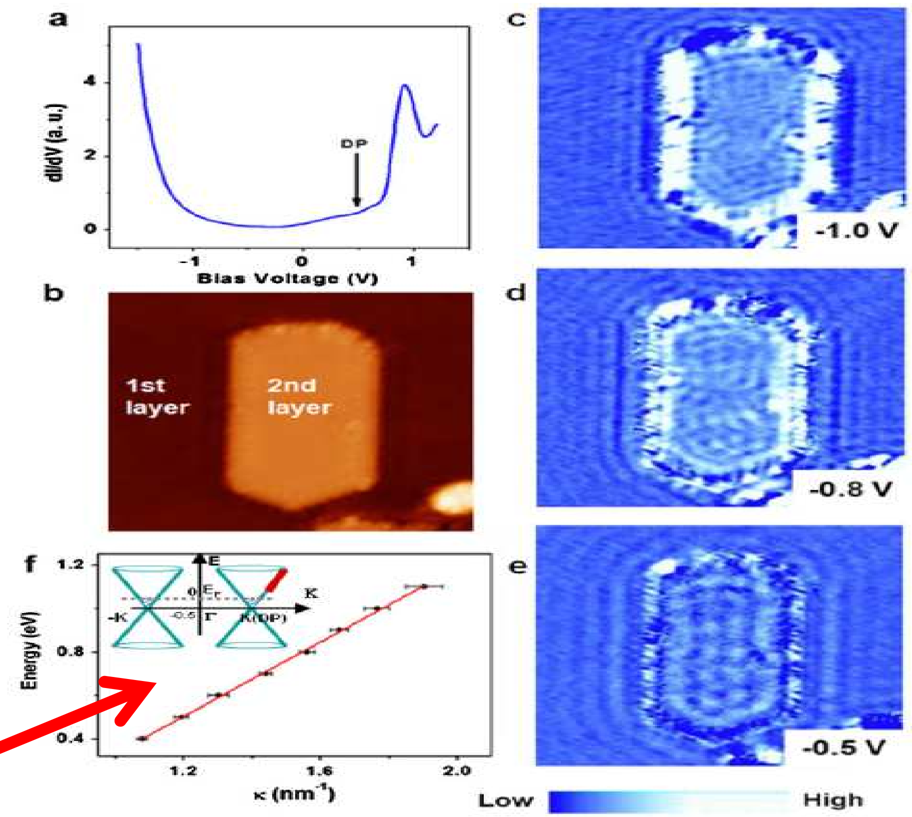


FIG. 4 (color online). (a) dI/dV curves taken at 77 K. The position of the DP is labeled. (b) The STM image (40 nm × 40 nm) of the 1 ML silicene surface containing an island of second layer taken at tip bias −1.0 V. (c), (d), and (e) dI/dV maps of the same area as (b) taken at tip bias −1.0, −0.8, and −0.5 V, respectively. (f) Energy dispersion as a function of κ for silicene determined from the wavelength of QPI patterns. The inset shows a schematic drawing of the overall band structure, with the relative location of the DP, E_F, and our data points [red (thick gray) line].

Linear dispesion

Dirac cone

Lan Chen et al. PRL 109, 056804 (2012)

Silicene sheet:

Si/Ag(111)

Electronic properties (STS)

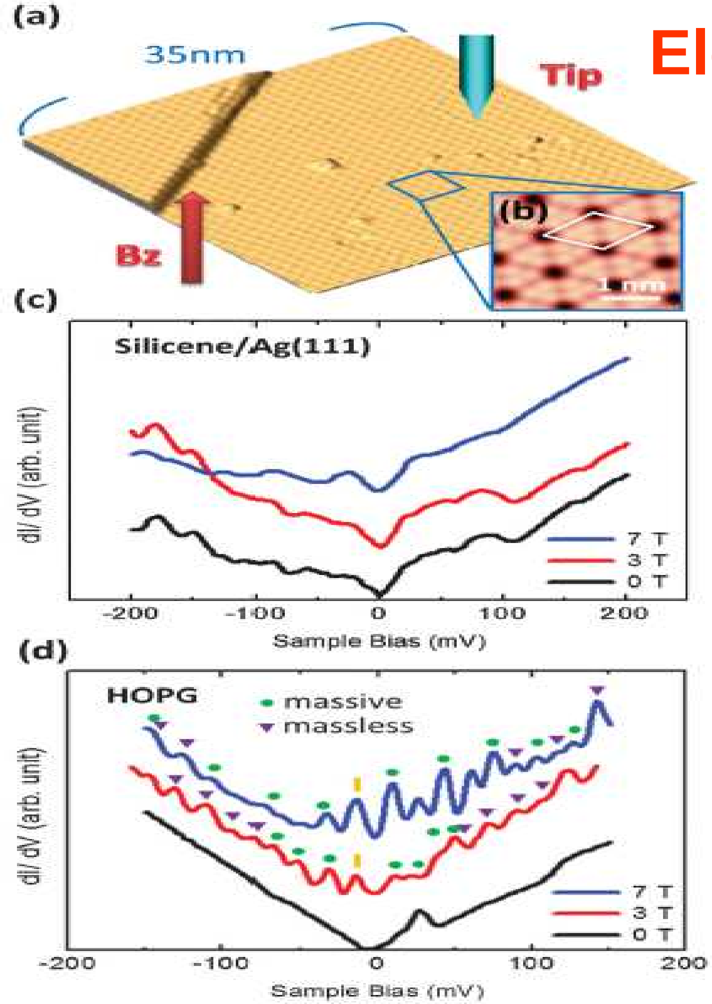


FIG. 1 (color). (a) STM image of large area of silicene (sample bias voltage $V_s = -0.70$ V and tunneling current $I_t = 0.19$ nA. The image size is 35×35 nm^2.) (b) High resolution STM image of the 4×4 silicene ($V_S = +0.50$ V and $I_t = 0.30$ nA, 3.65×3.65 nm^2). The unit cell is shown by the white rhombus. (c) The STS spectra of silicene for various magnetic fields perpendicular to the sample surface, B_z. (d) The STS spectra of HOPG for various B_Z. The purple triangles and green circles show the peaks originating from the LLs of massless and massive Dirac fermions, respectively. The $n = 0$ LL is marked by the yellow bar and the $n = 1$ LL of massive Dirac fermions is not clearly resolved in 3 T due to low magnetic field.

No linear dispersion !!!

Dirac cone

Chun-Liang Lin etal. PRL 110, 076801 (2013)

Silicene sheet:

Si/Ag(111)

PHYSICAL REVIEW B **87**, 245430 (2013)

Absence of a Dirac cone in silicene on Ag(111): First-principles density functional calculations with a modified effective band structure technique

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We investigate the currently debated issue of the existence of the Dirac cone in silicene on an Ag(111) surface, using first-principles calculations based on density functional theory to obtain the band structure. By unfolding the band structure in the Brillouin zone of a supercell to that of a primitive cell, followed by projecting onto Ag and silicene subsystems, we demonstrate that the Dirac cone in silicene on Ag(111) is destroyed. Our results clearly indicate that the linear dispersions observed in both angular-resolved photoemission spectroscopy [P. Vogt *et al.*, Phys. Rev. Lett. **108**, 155501 (2012)] and scanning tunneling spectroscopy [L. Chen *et al.*, Phys. Rev. Lett. **109**, 056804 (2012)] come from the Ag substrate and not from silicene.

No Dirac cone

Y. Peng et al. Phys. Rev. B. 87 245430 (2013)

Silicene sheet:

Si/Ag(111)

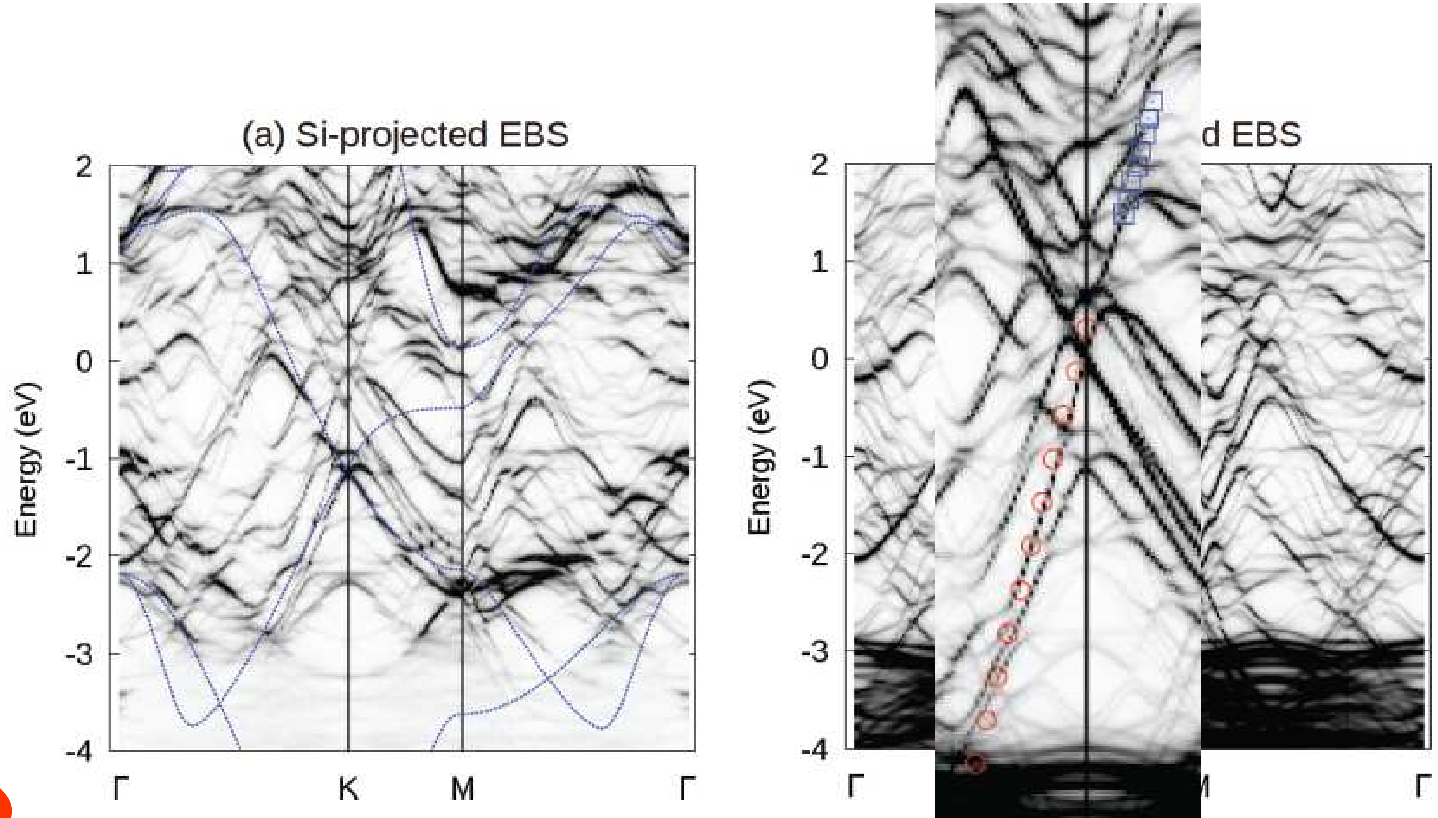


FIG. 2. (Color online) Si- and Ag-projected effective band structure (EBS) of the silicene-Ag system. (a) Si-projected effective band structures, with band structure of standalone low-buckled silicene plotted as blue dashed lines. Note that the band structure of low-buckled silicene was shifted downward by 1.1 eV. (b) Ag-projected effective band structures with experimental observed linear dispersions (red circles: measurements from Ref. 7, blue squares: measurements from Ref. 8).

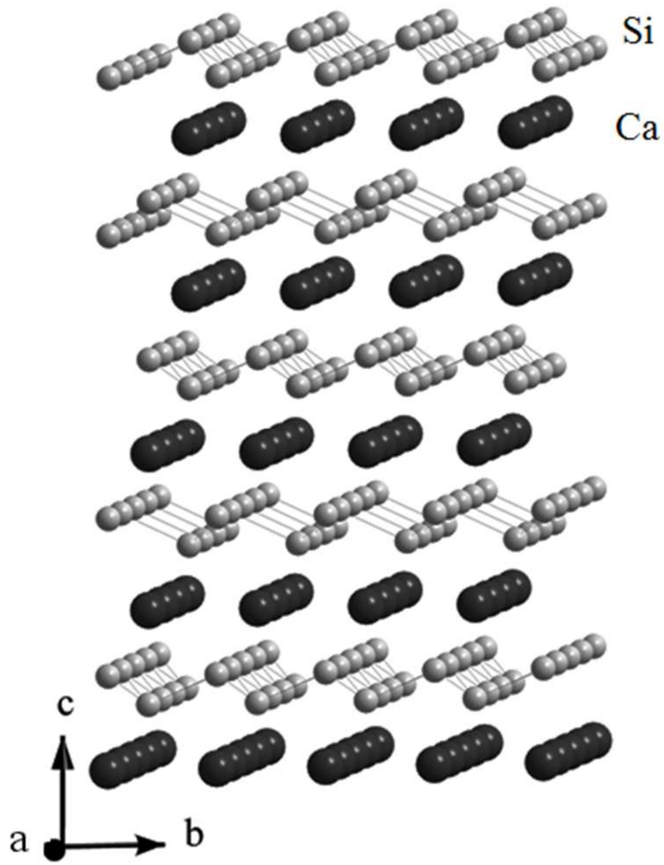
No Dirac cone

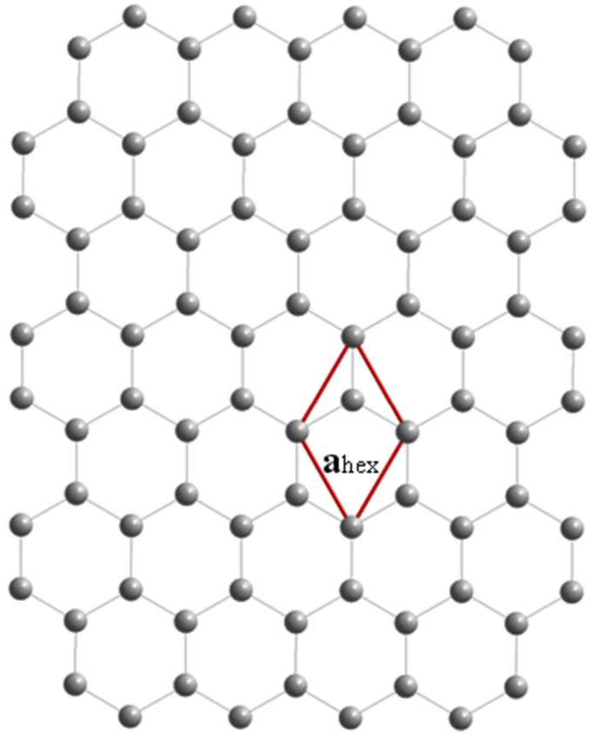
Y. Peng et al. Phys. Rev. B. 87 245430 (2013)

Future challenges

Chemical Synthesis

$CaSi_2$





Future challenges

Chemical Synthesis

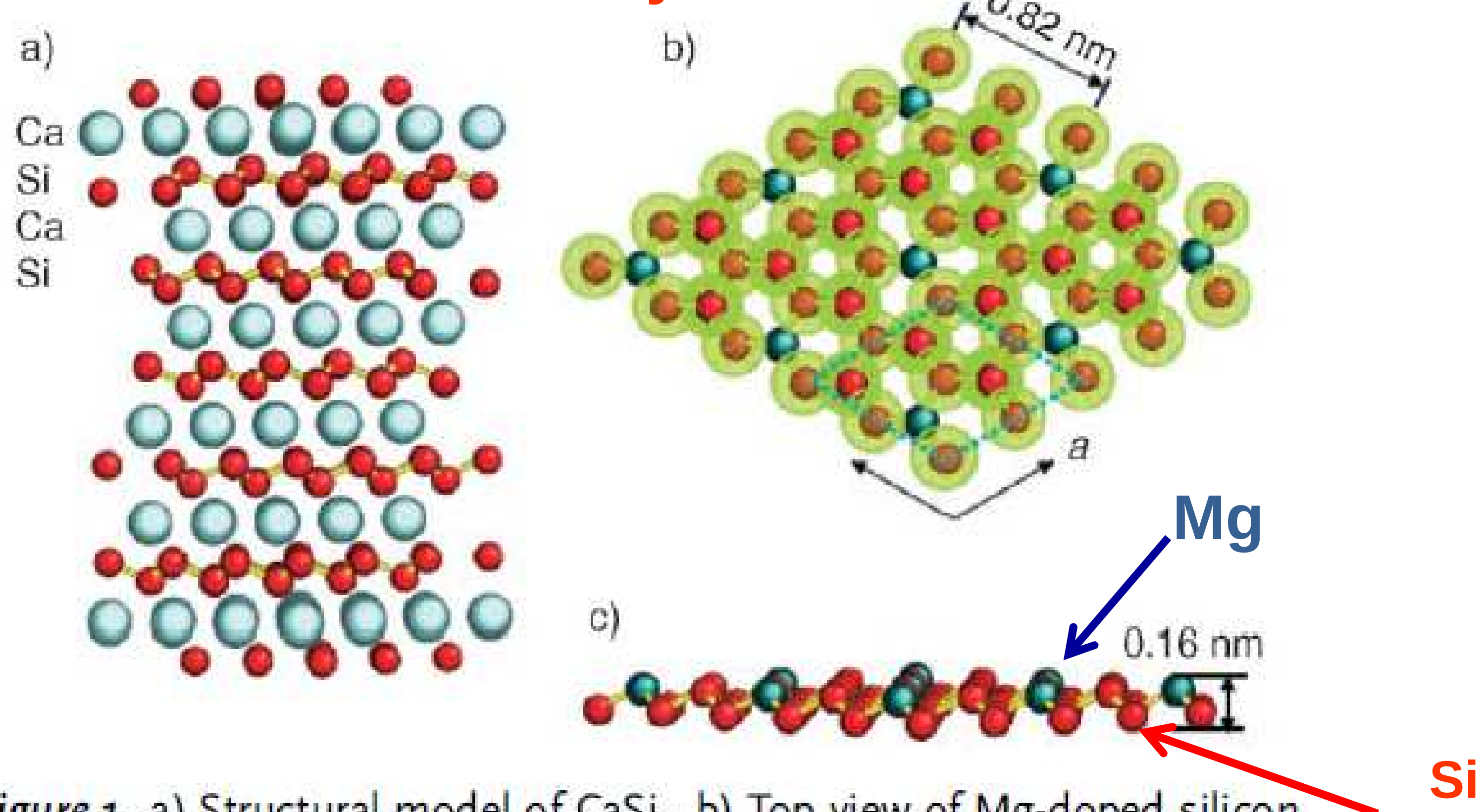


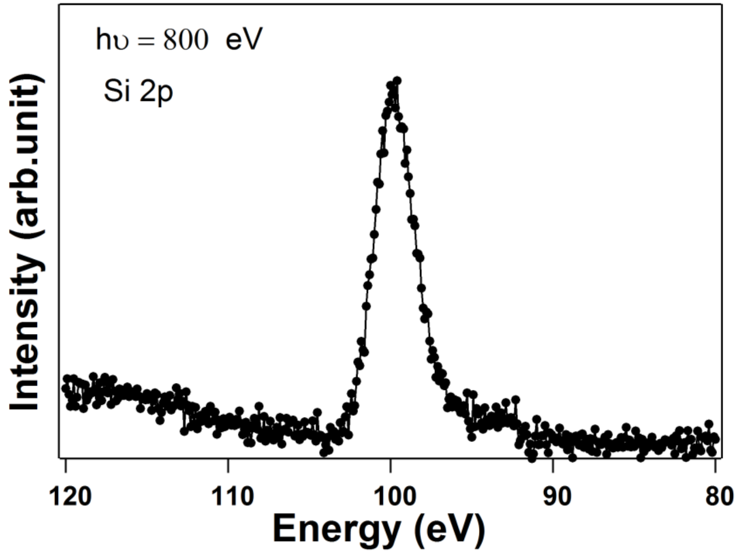
Figure 1. a) Structural model of $CaSi_2$. b) Top view of Mg-doped silicon sheet capped with oxygen; the axis notation follows that for the hexagonal crystal structure of the parent layered silicon. c) Side view of the core of the silicon sheet; the large yellow-green circles represent oxygen atoms, small red (Si) and green (Mg) circles represent the Si(111) plane in the layer below.

H. Nakano et al. Angew.Chzem. 2006, 118 6451-6454

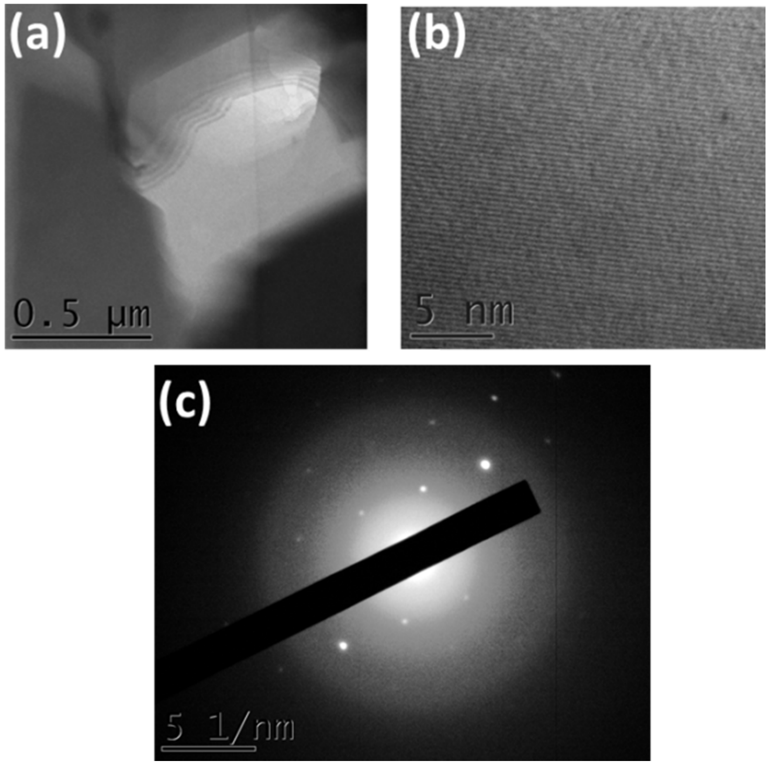
Chemical Synthesis

SILICON SHEETS BY REDOX ASSISTED CHEMICAL EXFOLIATION

PES



TEM



Silicon with graphitic structure

M. R. TCHALALA J. Phys.: Condens. Matter, 25, 442001 (2013)

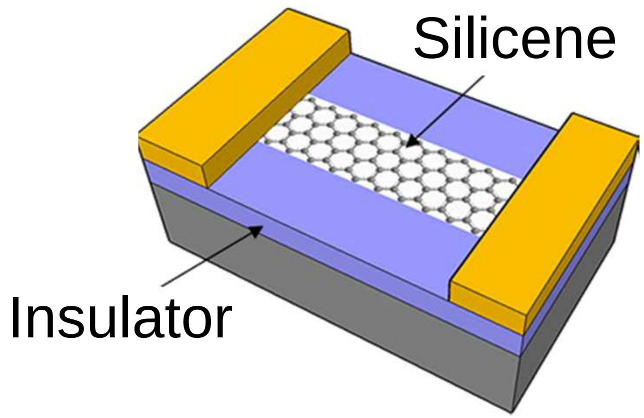
Future challenges

Silicene growth and transferability

- How to grow silicene on large scale-area on insulators ?

- Can we control the interaction of silicene with its supporting substrate for transferablity ?

- Synthesis by chemical methods ?



Conclusion

- Experimental evidence of Silicene on different substrates (Nano-ribbons and sheet)

- Electronic properties of silicene still under debate

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