

Investigation of corrosion by means of adsorption energy analysis in DFT simulations



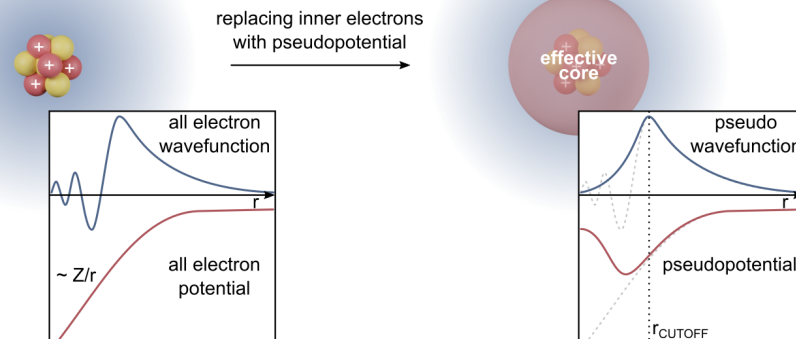
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Density Functional Theory

- Method is based on the Hohenberg-Kohn Theorems
- Calculations are carried out using Kohn-Sham equations
- Electron structure is assessed by means of the potential acting on the electrons
- Potential depends solely on the type and arrangement of the atoms in the structure
- Projector-Augmented Wave (PAW) method – based on Ultra-soft pseudo-potential
- Full all-electron wave functions and density
- Efficient and accurate



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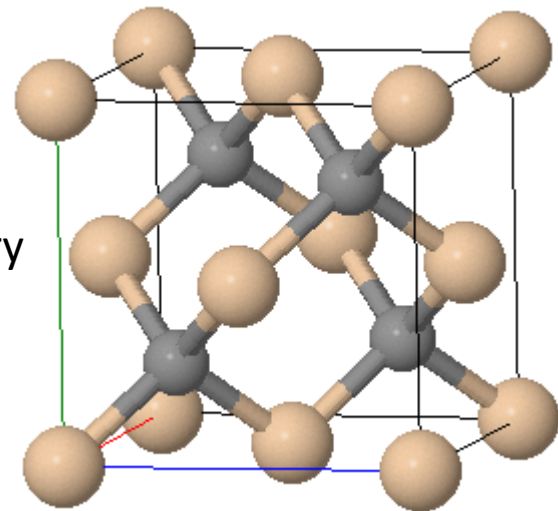


Studied cases

- 3C-SiC (β -SiC) highest electron mobility, saturation velocity and lowest Band gap (2.3eV) in all polytypes
- Zincblende structure - FCC

Commonly occurring surfaces

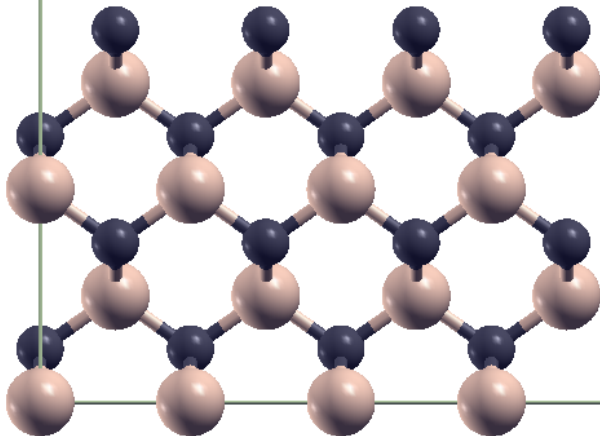
- 100 Surface – parallel to front surface, 4 fold symmetry
- 111 Surface – plane intersecting x, y, z axes, 6 fold symmetry
- 110 Surface – plane intersecting x, y axes, 2 fold symmetry



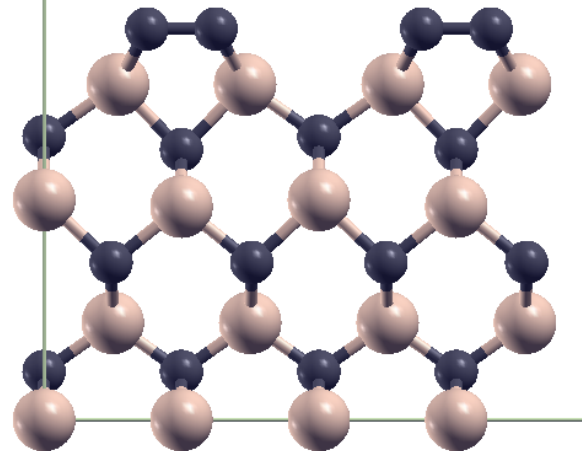
100 Surface C- face

- C-C distance 1.36 Å
- Si-C 1.84 Å (1.66 in bulk crystal)
- Final energy = -4162.857 Ry

Initial position

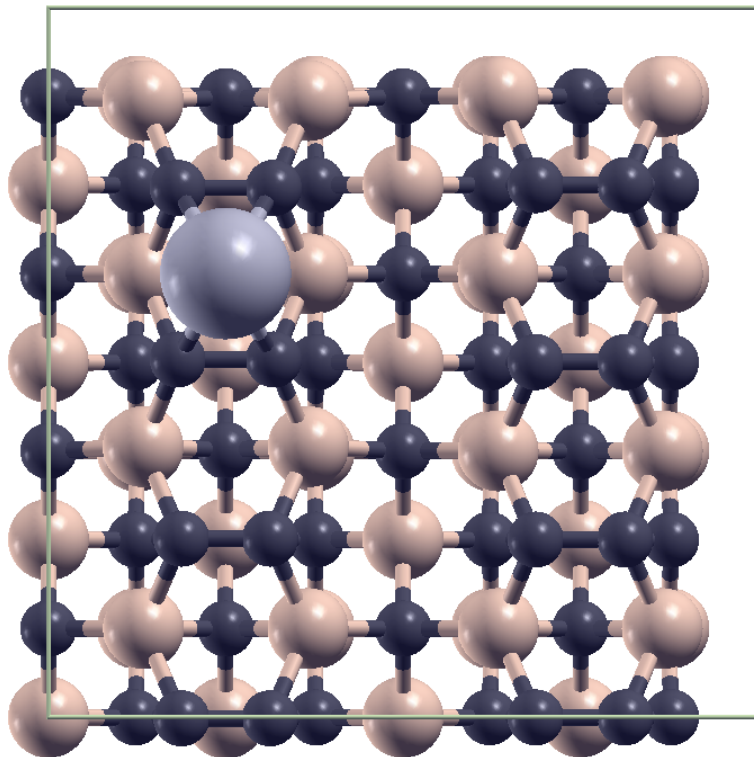


Final position





100 Surface



- Pb-C distance 2.48 Å
- Final energy = -5033.472 Ry
- Adsorption energy calculation:

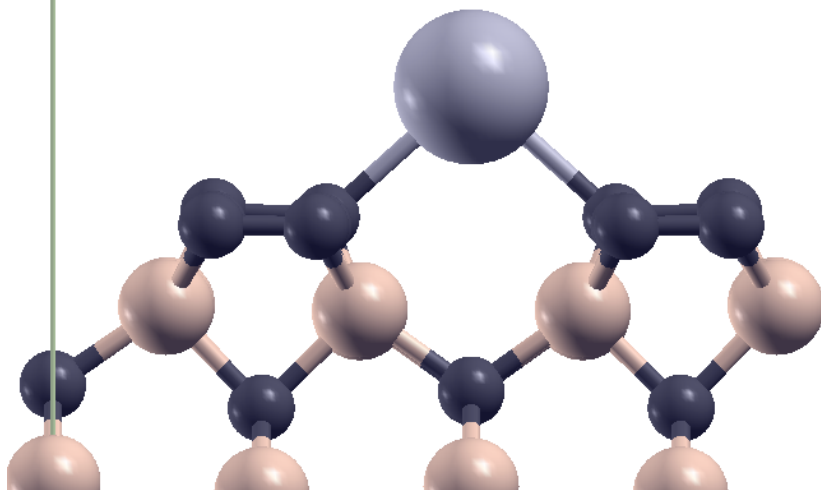
$$E_{\text{adsorption}} = [E_{\text{system}} - (E_{\text{adsorbent}} + E_{\text{adsorbate}})]$$

$$E_{\text{adsorbate(Pb)}} = -870.23 \text{ Ry}$$

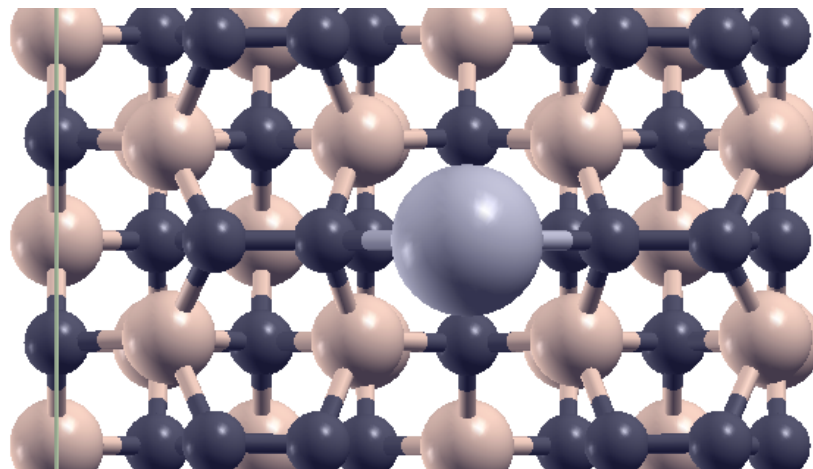
- $E_{\text{adsorption}} = -5.23 \text{ eV}$



100 Surface

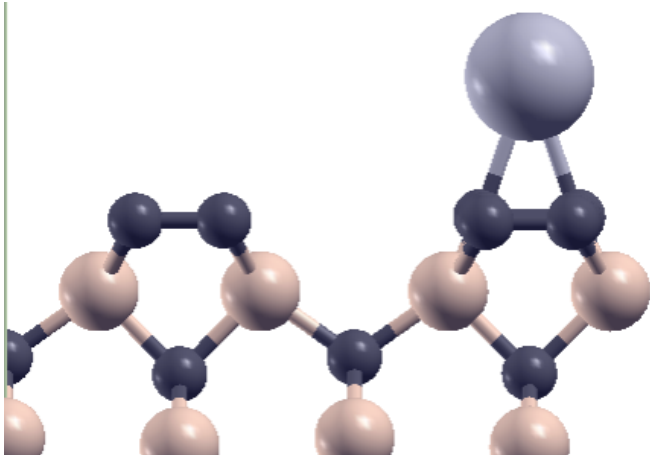


- Pb-C distance 2.52 Å
- Final energy = -5033.439 Ry
- $E_{\text{adsorption}} = -4.78 \text{ eV}$

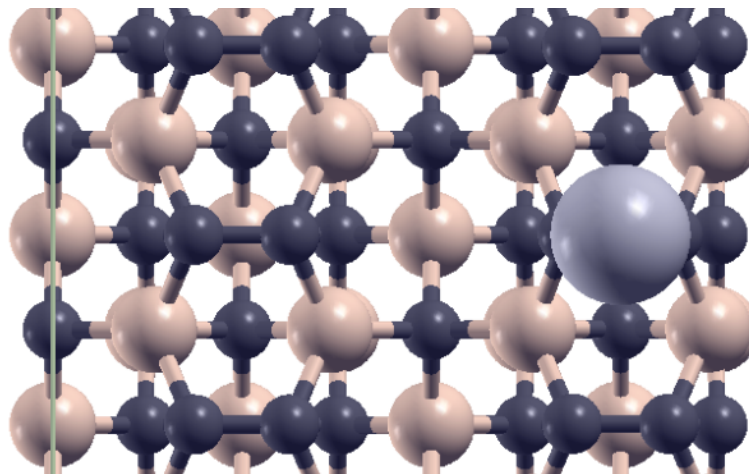




100 Surface



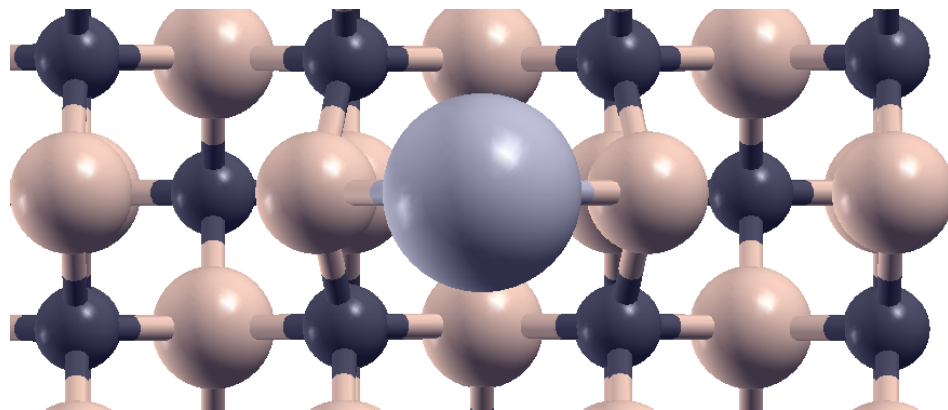
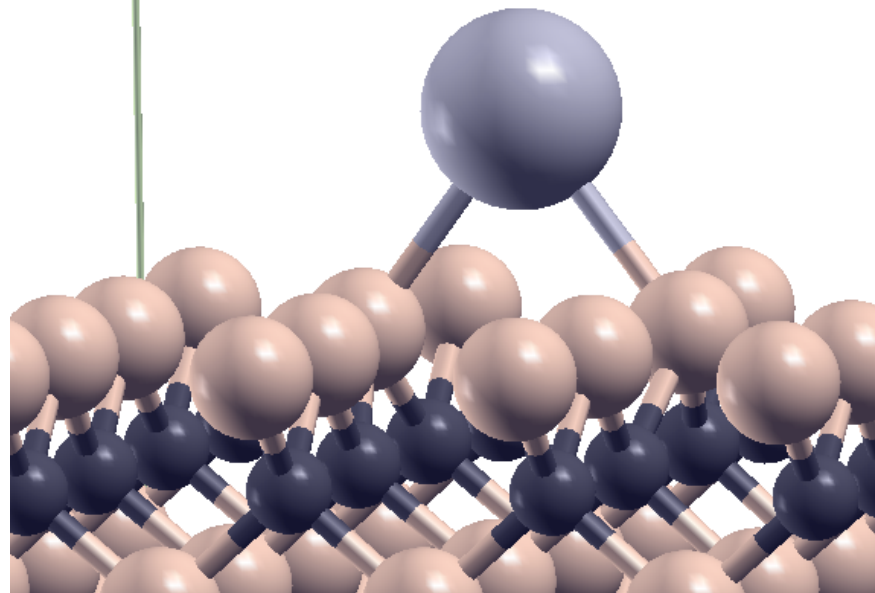
- Pb-C distance 2.30 Å
- Final energy = -5033.440 Ry
- $E_{\text{adsorption}} = -4.8 \text{ eV}$





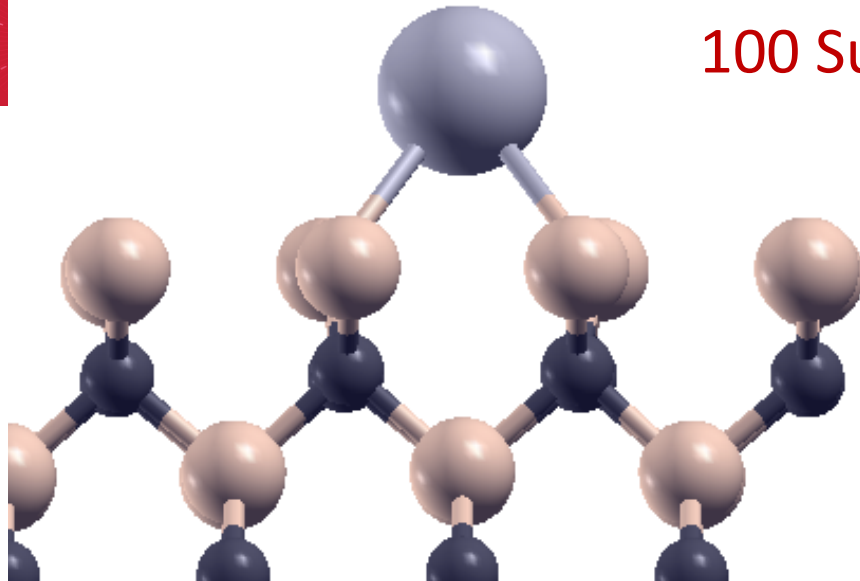
100 Surface Si-face

- Final $E_{\text{adsorbent}} = -4160.736$
- Pb-Si distance 2.77 \AA
- Final energy = -5031.348 Ry
- $E_{\text{adsorption}} = -5.19 \text{ eV}$

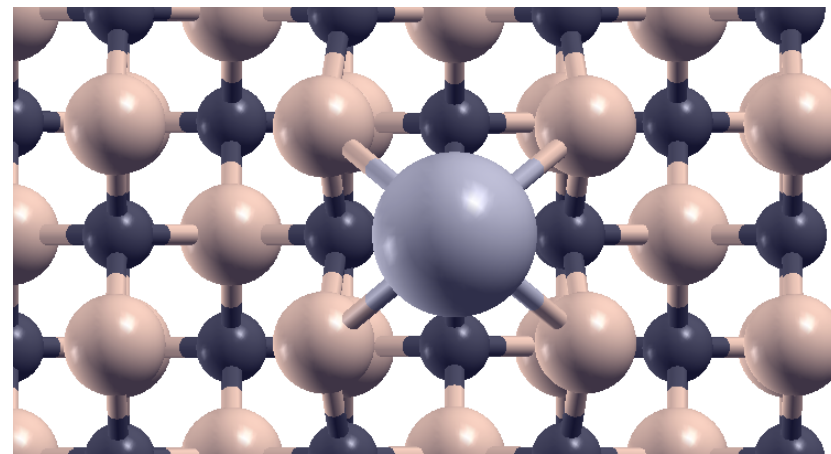




100 Surface

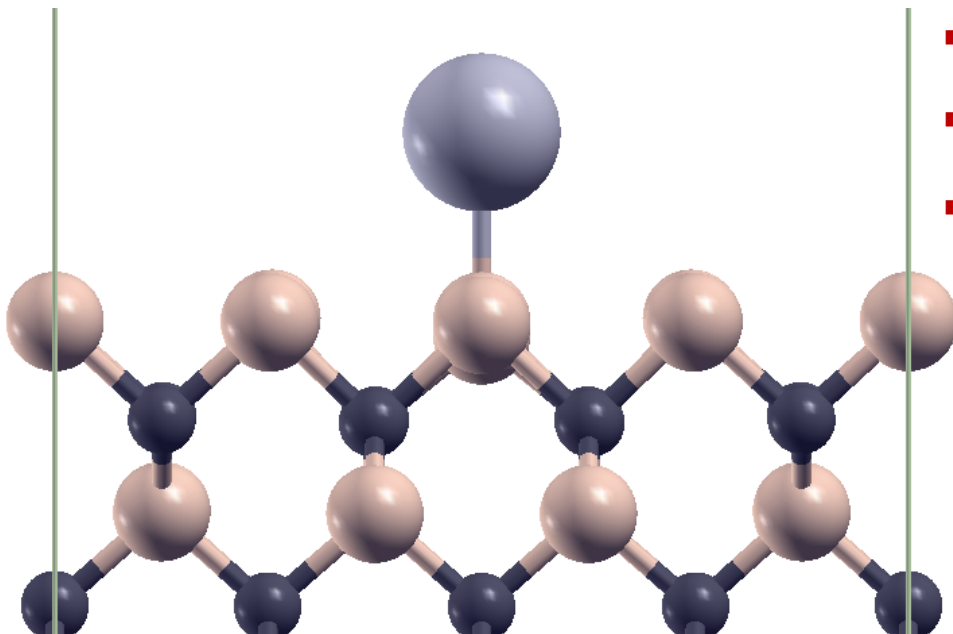


- Pb-Si distance 2.95 Å
- Final energy = -5031.378 Ry
- $E_{\text{adsorption}} = -5.6 \text{ eV}$





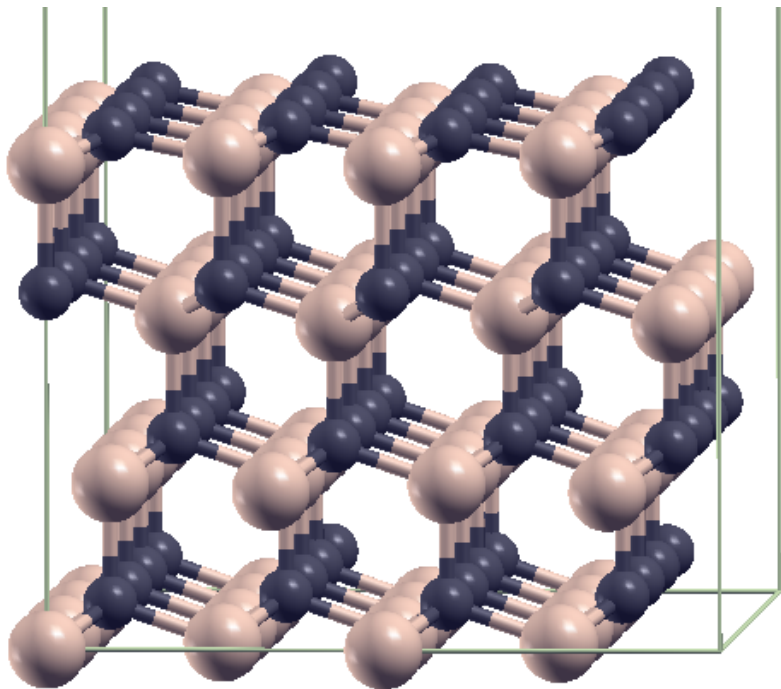
100 Surface



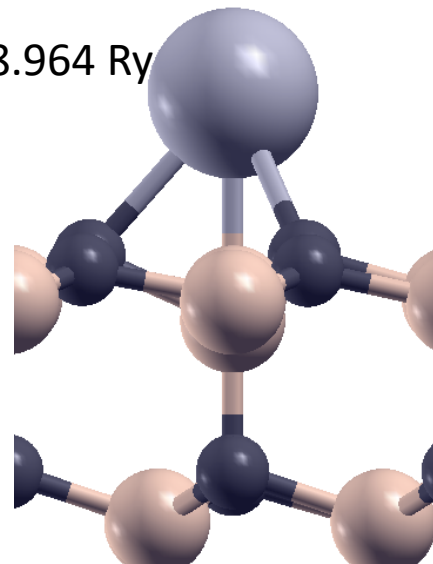
- Pb-Si distance 2.57 Å
- Final energy = -5031.272 Ry
- $E_{\text{adsorption}} = -4.16 \text{ Ry}$



111 Surface C-face

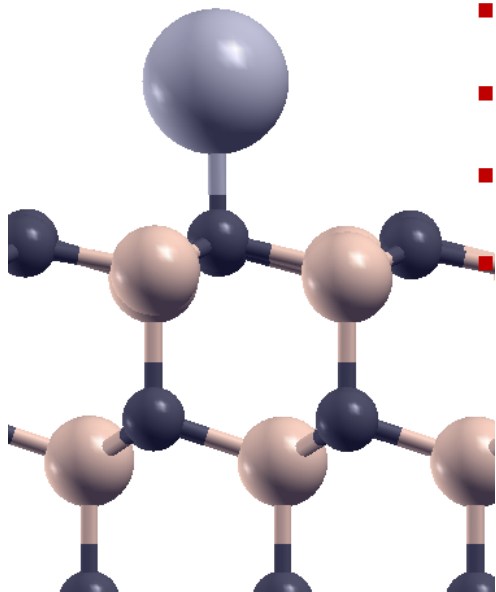


- Final $E_{\text{adsorbent}} = -4168.232 \text{ Ry}$
- Pb-Si distance 2.67 \AA
- Pb-C distance 2.55 \AA
- Final energy = -5038.964 Ry
- $E_{\text{adsorption}} = -6.82 \text{ eV}$



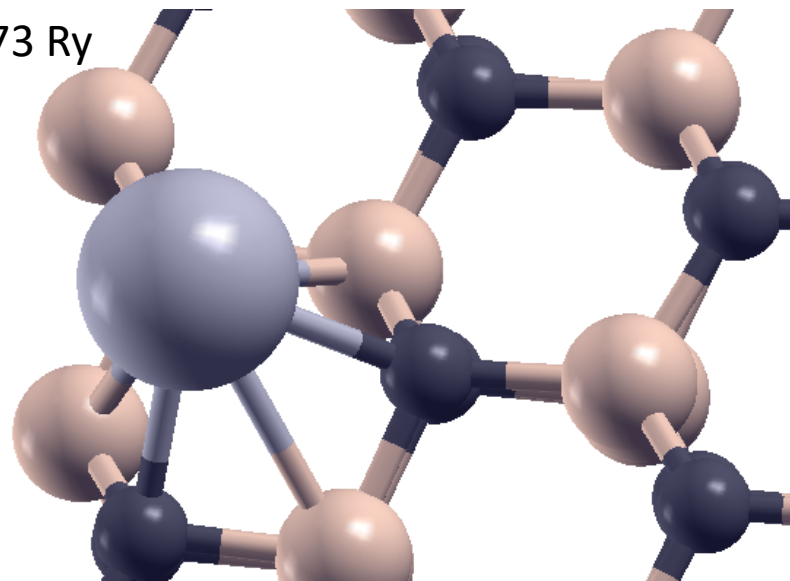


111 Surface



Initial position

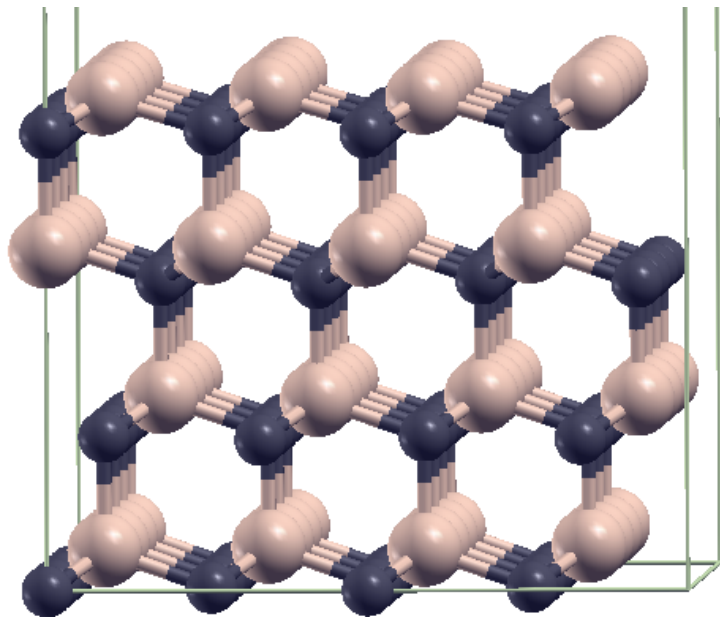
- Pb-Si distance 3.04 Å
 - Pb-C distance 2.53 Å
 - Final energy = -5038.973 Ry
- $E_{\text{adsorption}} = -6.95 \text{ eV}$



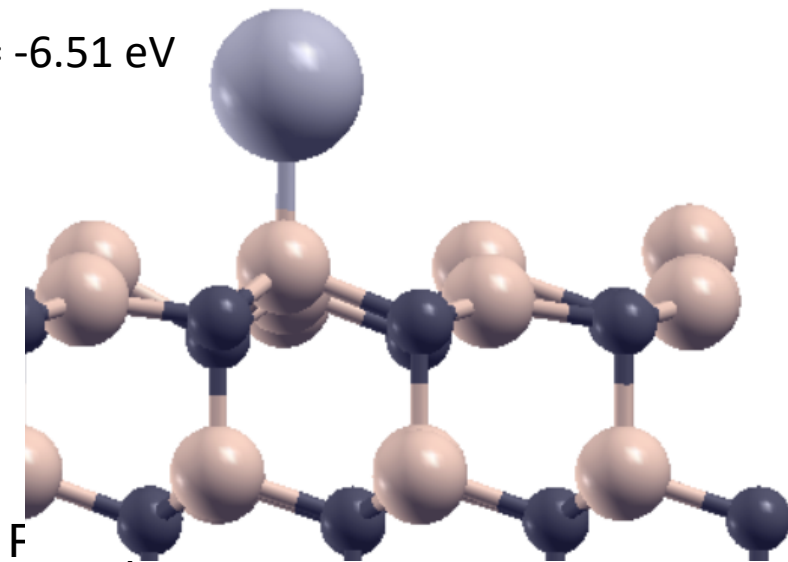
Final position



111 Surface Si-face

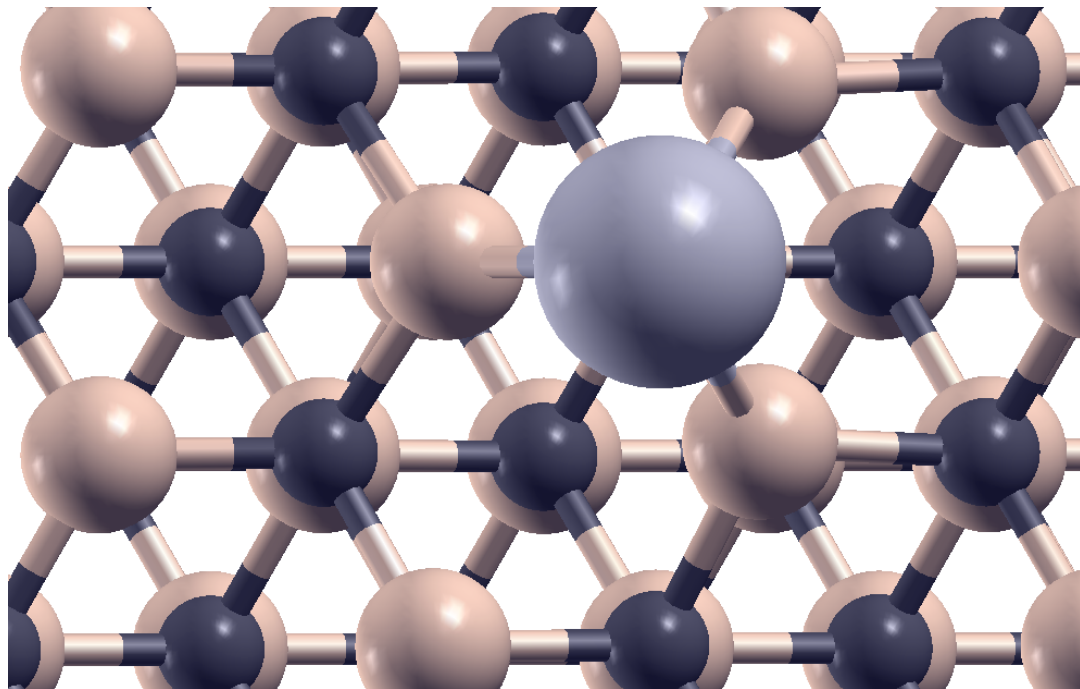


- Final $E_{\text{adsorbent}} = -4167.902 \text{ Ry}$
- Pb-Si distance 2.64 \AA
- Final energy = -5038.611 Ry
- $E_{\text{adsorption}} = -6.51 \text{ eV}$





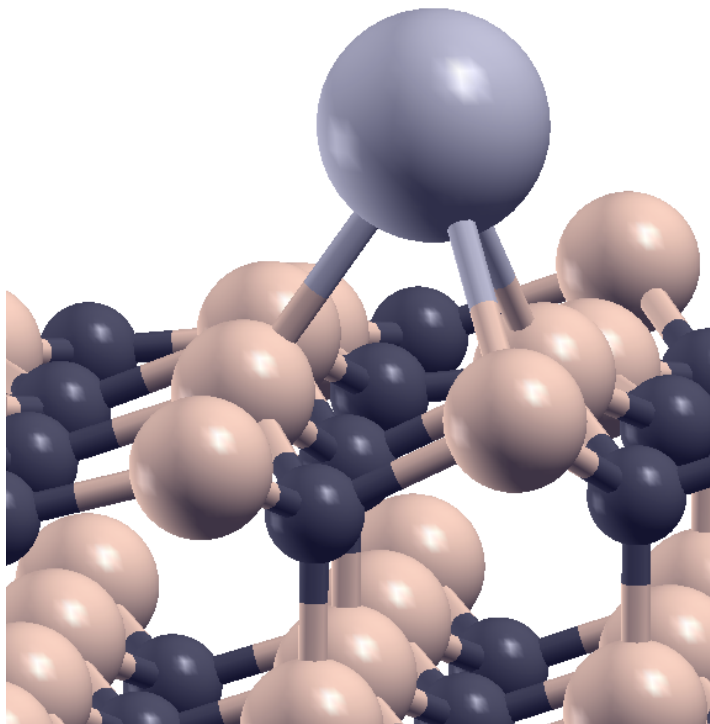
111 Surface



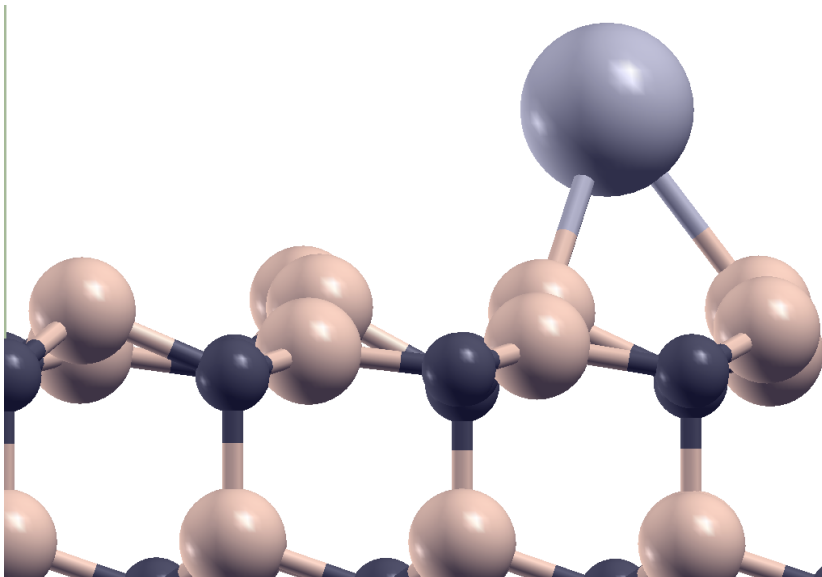
- Pb-Si distance 2.85, 2.87 Å
- Final energy = -5038.675 Ry
- $E_{\text{adsorption}} = -7.38 \text{ eV}$



111 Surface



- Pb-Si distance 2.85, 2.90 Å
- Final energy = -5038.667 Ry
- $E_{\text{adsorption}} = -7.27 \text{ eV}$





Summary

	100 Surface						111 Surface					
	C-face			Si-face			C-face			Si-face		
Position	gap	dimer	2 dimers	Si	2 Si	4 Si	Si	gap	gap	Si	gap	gap (C)
Energy [eV]	-4.78	-4.8	-5.23	-4.16	-5.19	-5.6	-6.82	-6.95	-6.95	-6.51	-7.27	-7.38

Lead ionization energy = 7.41 eV

- Shortest bond with lead is above C dimer on 100 surface – 2.30 Å
and longest in 111 C-face surface above interstitial site between Si – 3.04 Å
- Currently 110 Surface is simulated
- All relaxed structures will be calculated using:
Single-point (fixed-ion) SCF calculation with higher precision
with other Pseudo-potentials

Thank you for attention



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