



Università
degli Studi
di Ferrara

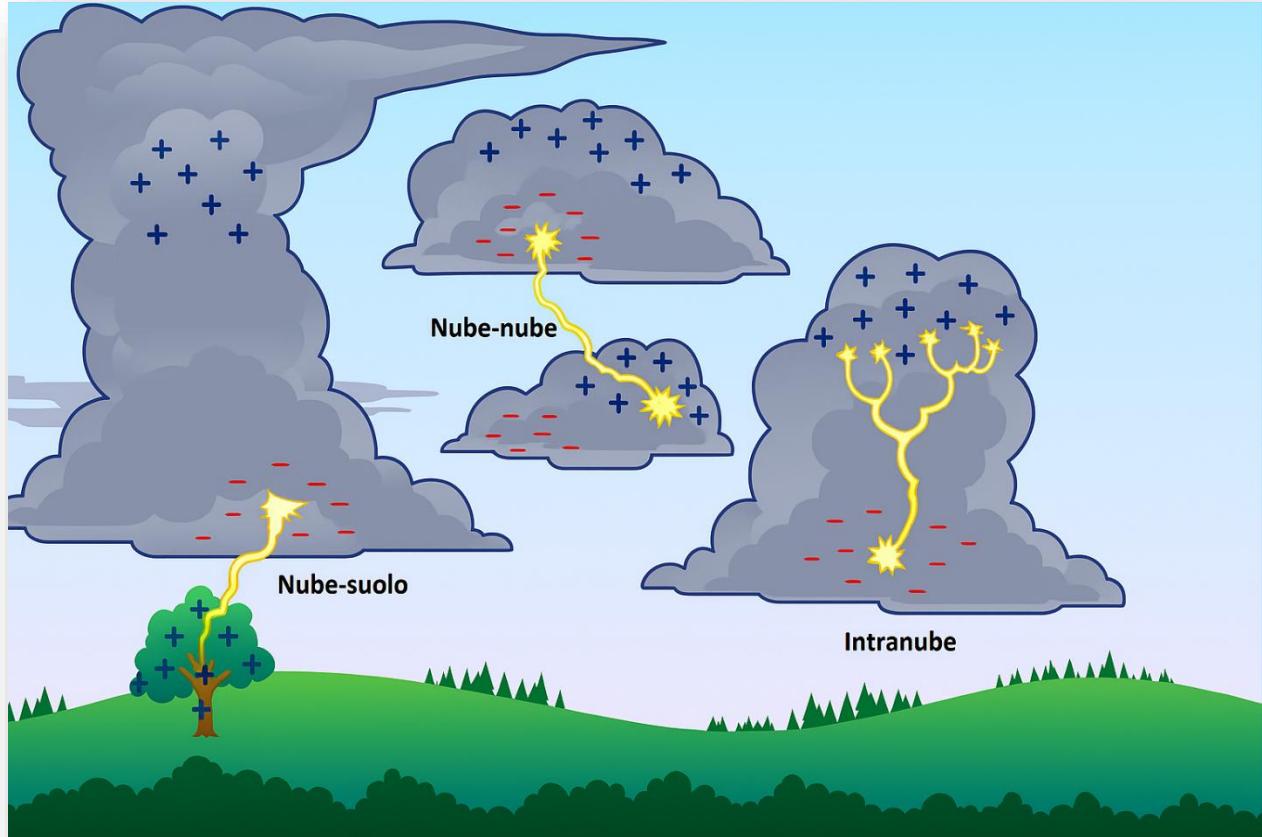
*Teoria fondamentale della triboelettrificazione di
intrusione/estruzione:
meccanismi chimici alla base della produzione di
corrente prodotta da contatto solido/liquido*

Relatore: Prof. Simone Meloni

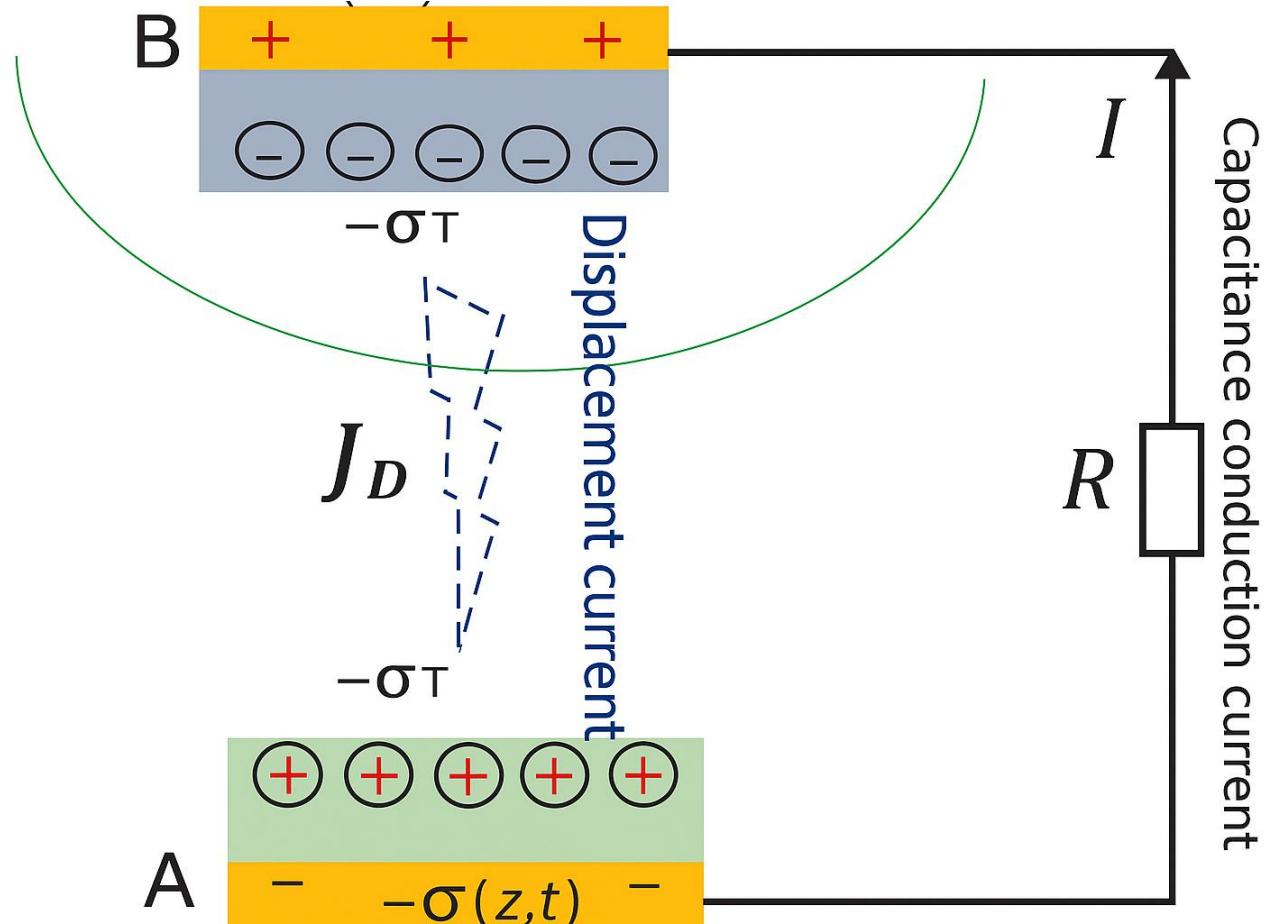
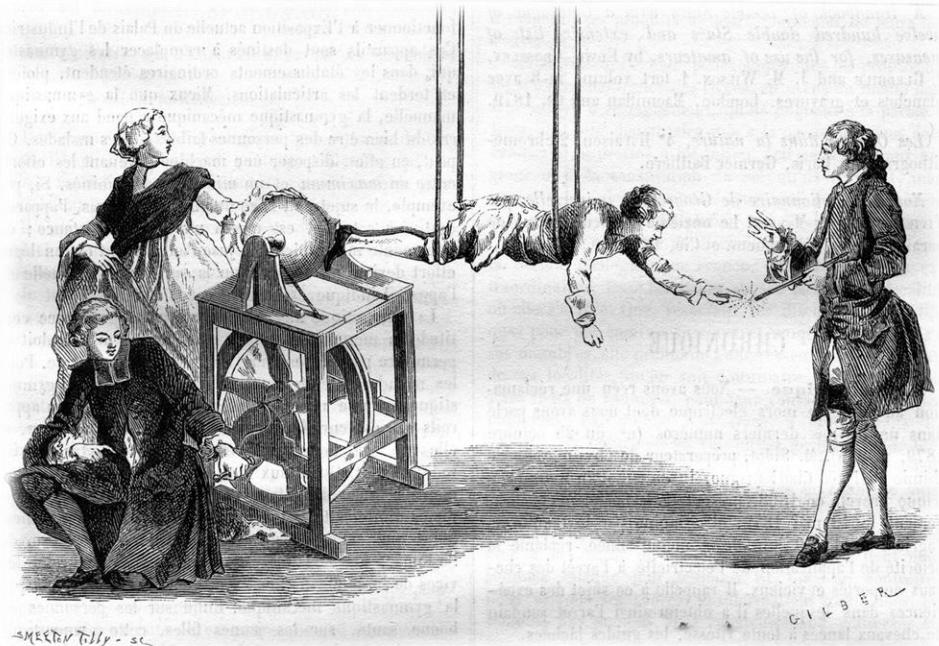
Correlatore: Dr. Nicola Verziaggi

Laureando:

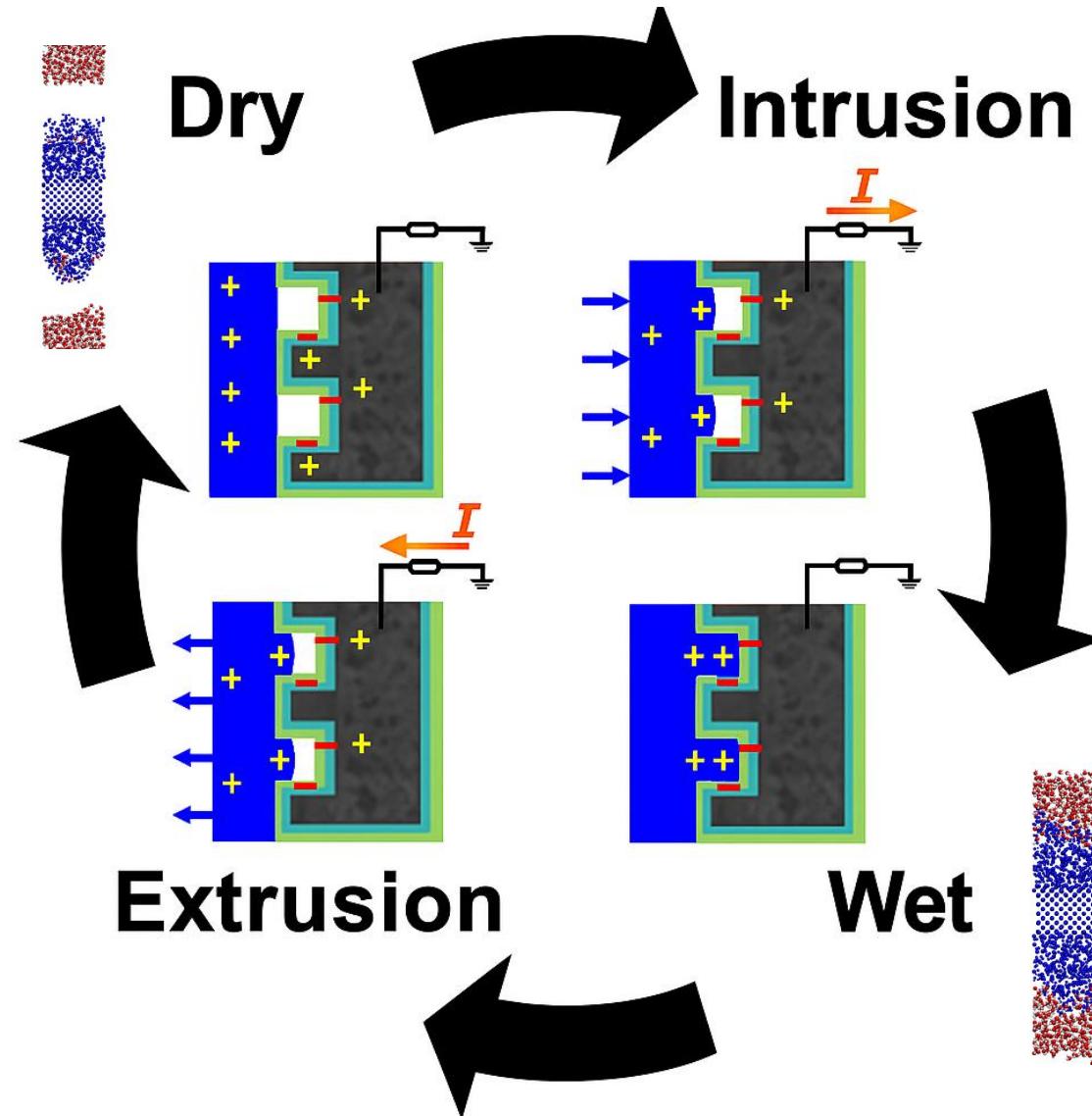
Leonardo Gnesato Anselmi



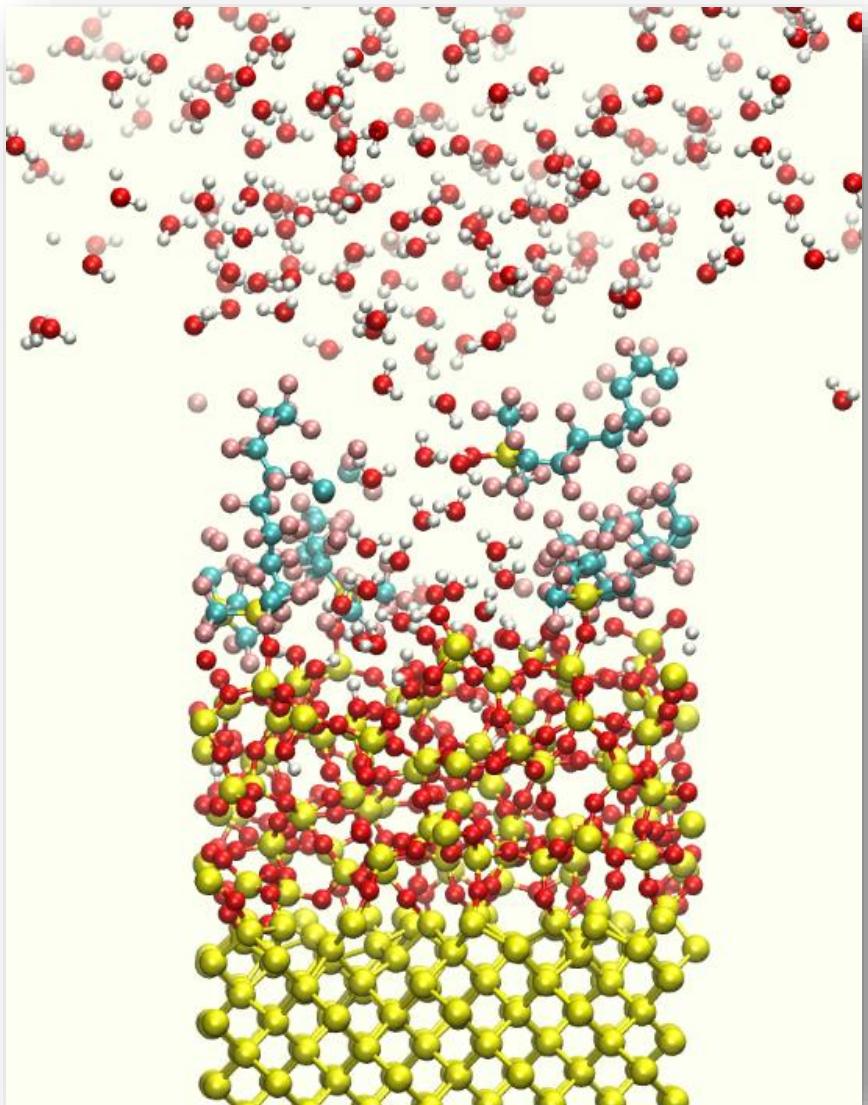
Triboelectric nano generators(TENG)



IE-TENGs(intrusion-extrusion triboelectric nano generators)

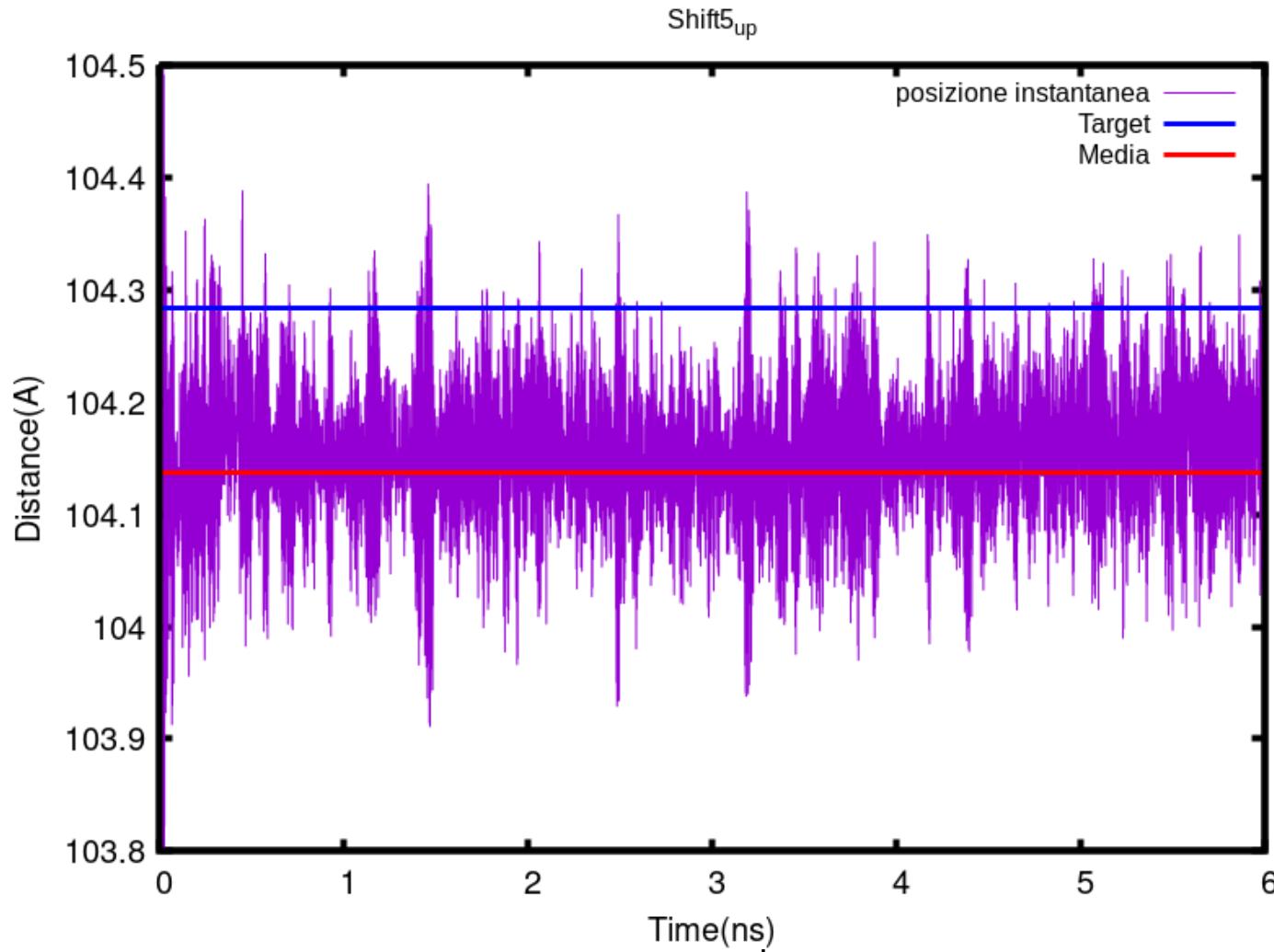


Let's rock chemistry in virtual space



- $Si^+ e [C8 - CF_3SiO]^-$
- $O^- e [C8 - CF_3Si]^+$
- *Nessuna carica*

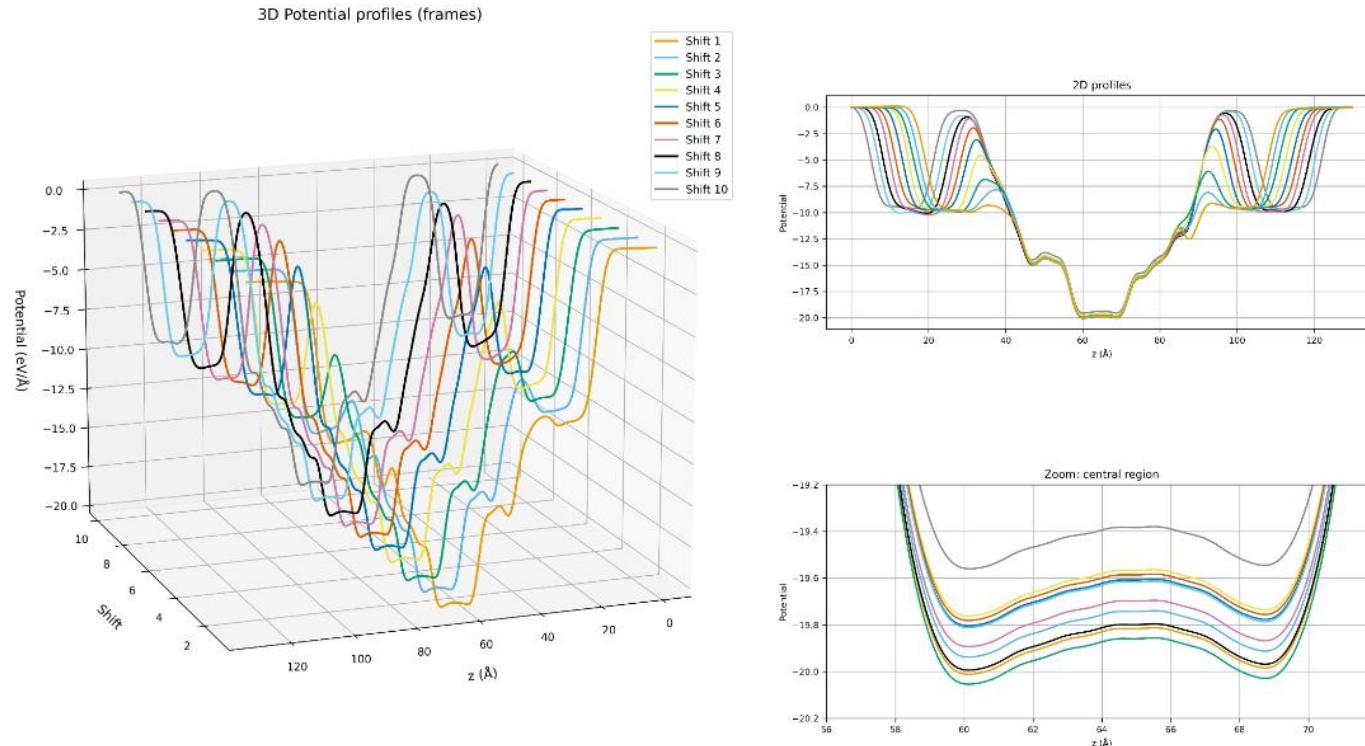
Analisi della fase di estrusione(RMD)



- LAMMPS
- Restrained molecular dinamycs
- Da intruso ad estruso
- *Variabile Shift*
- Forza esterna

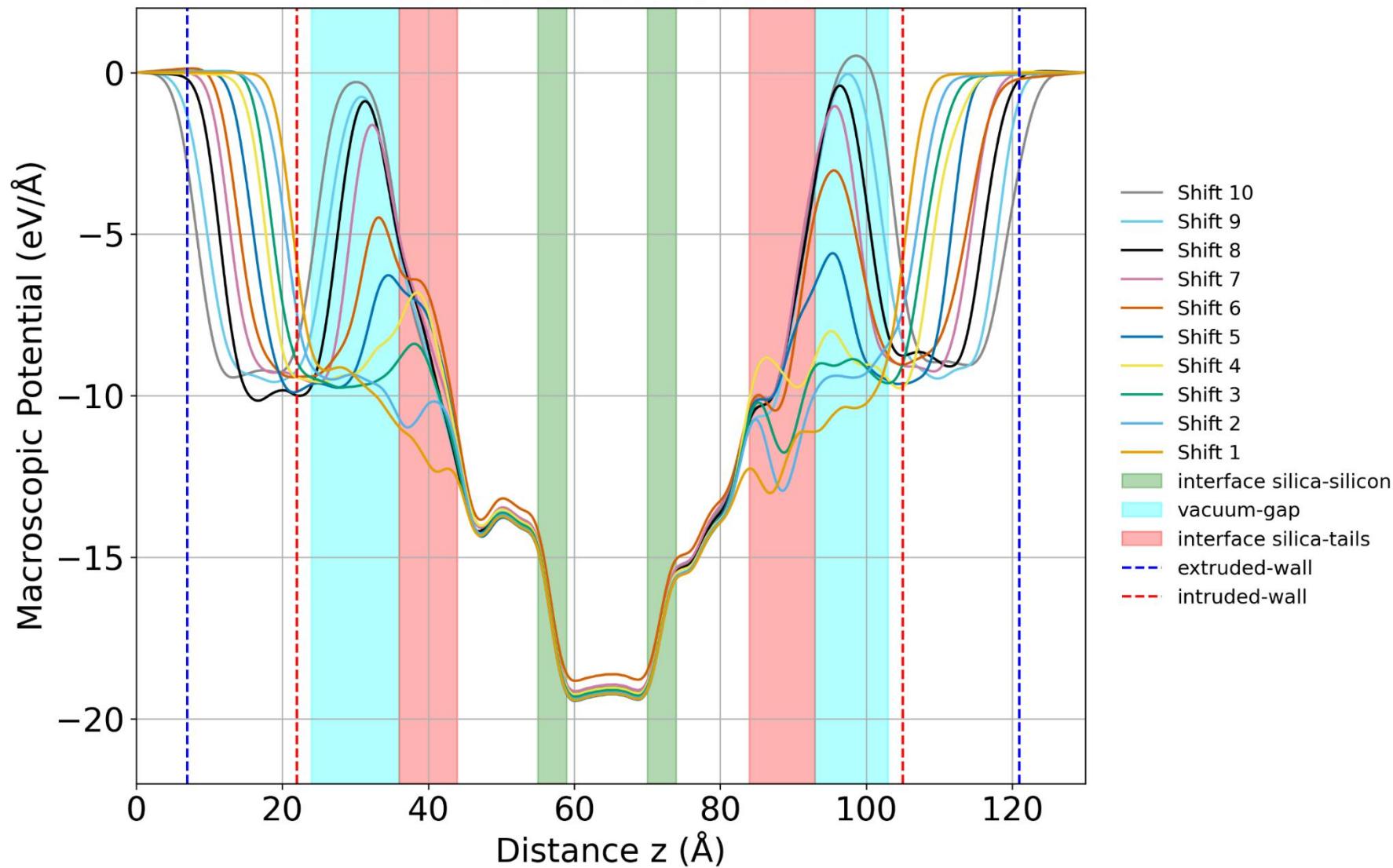
$$\mathbf{F} = -K(z(r) - z_{eq})$$

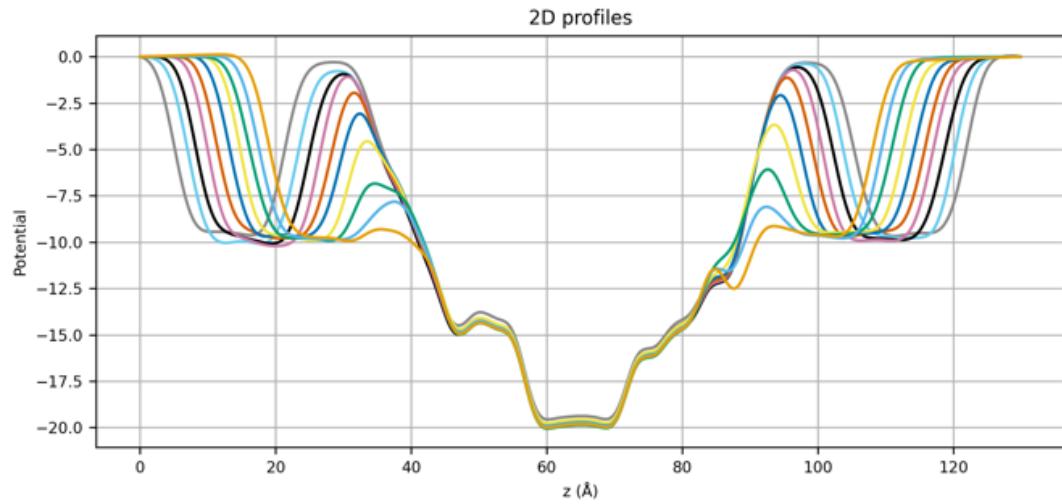
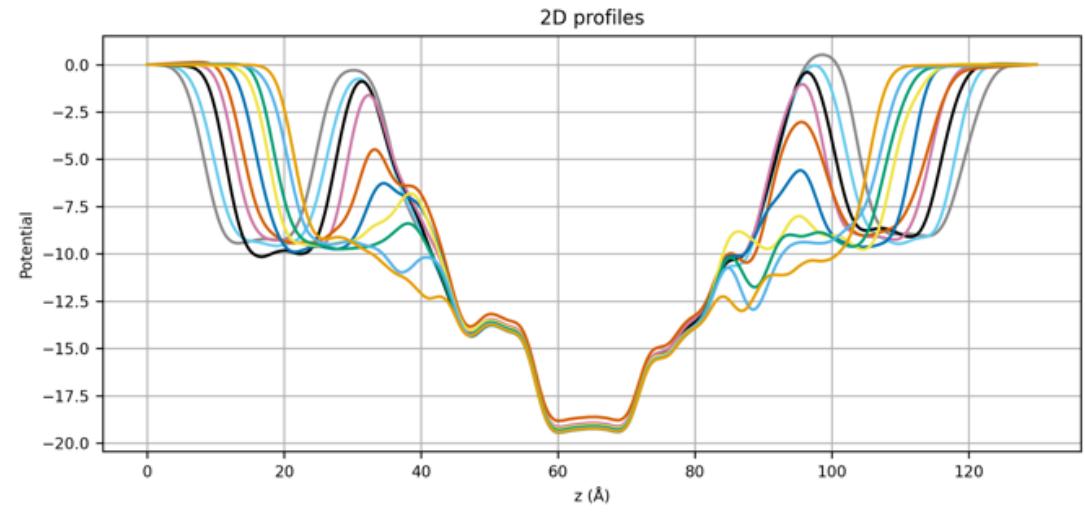
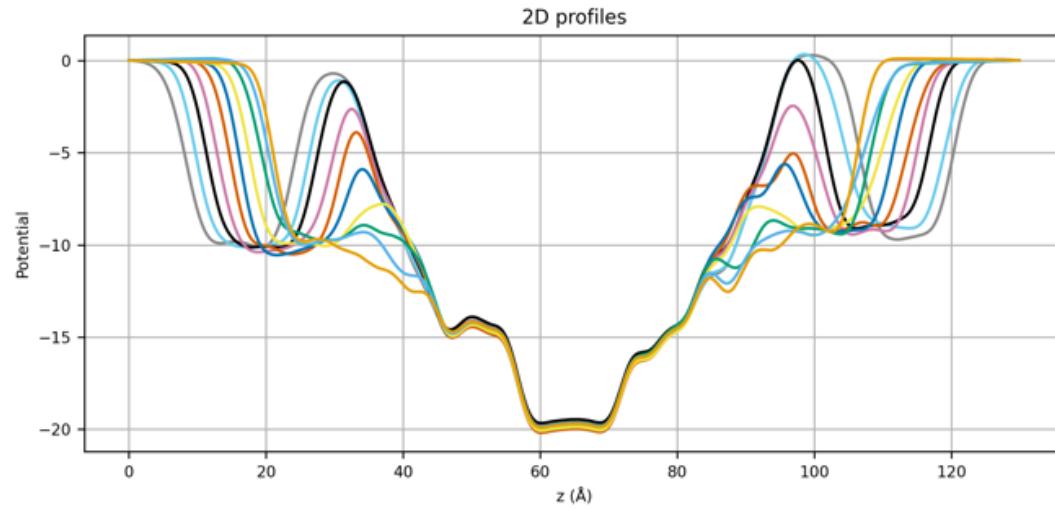
Procedimento computazionale



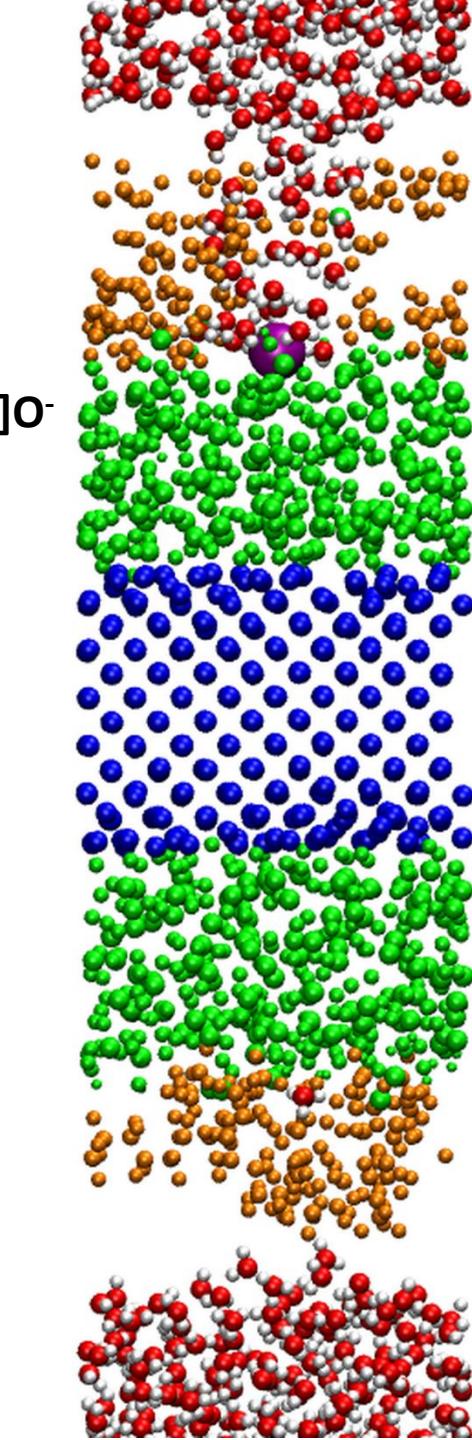
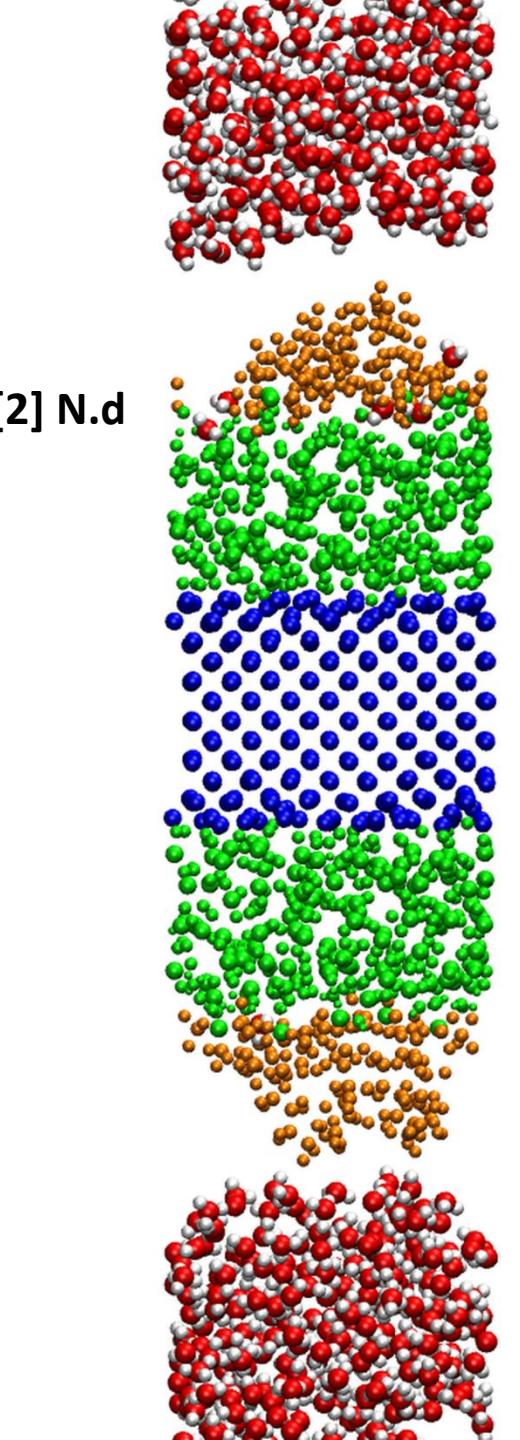
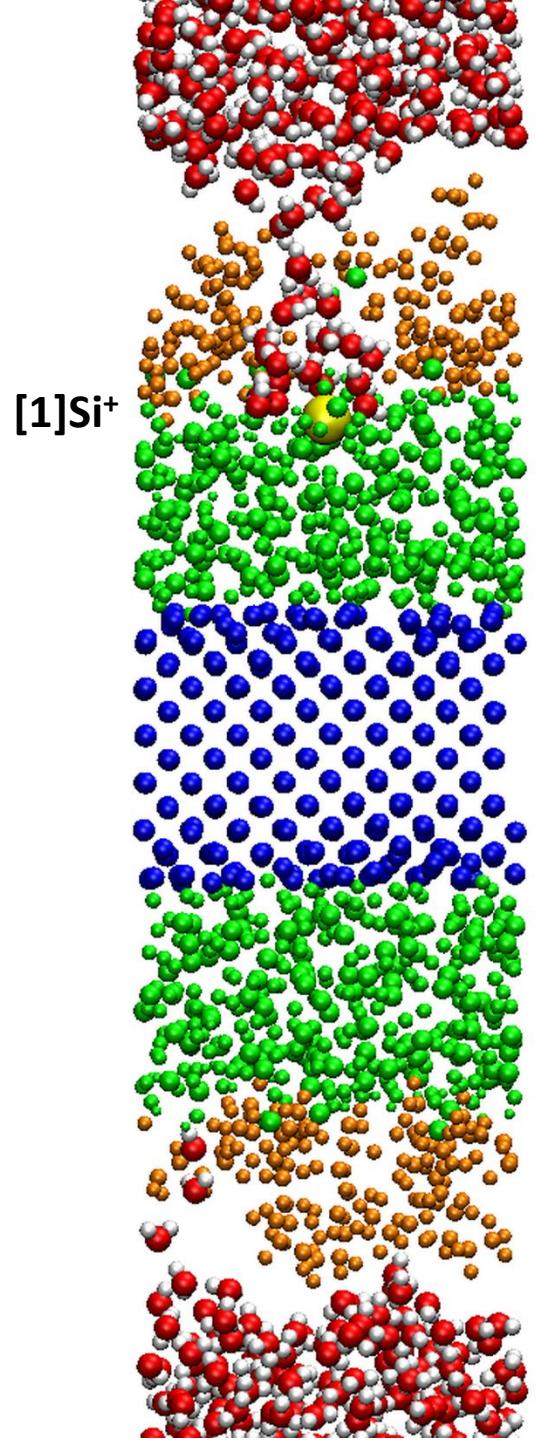
- Simulazioni 6 ns
- Immagini /frame
- VASP
- Potenziale elettrico macroscopico lungo z

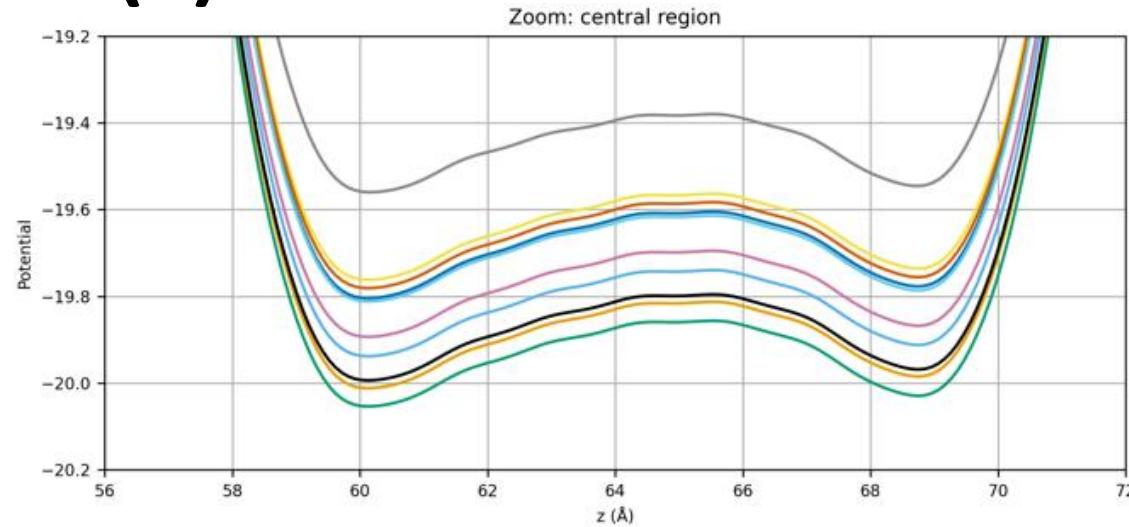
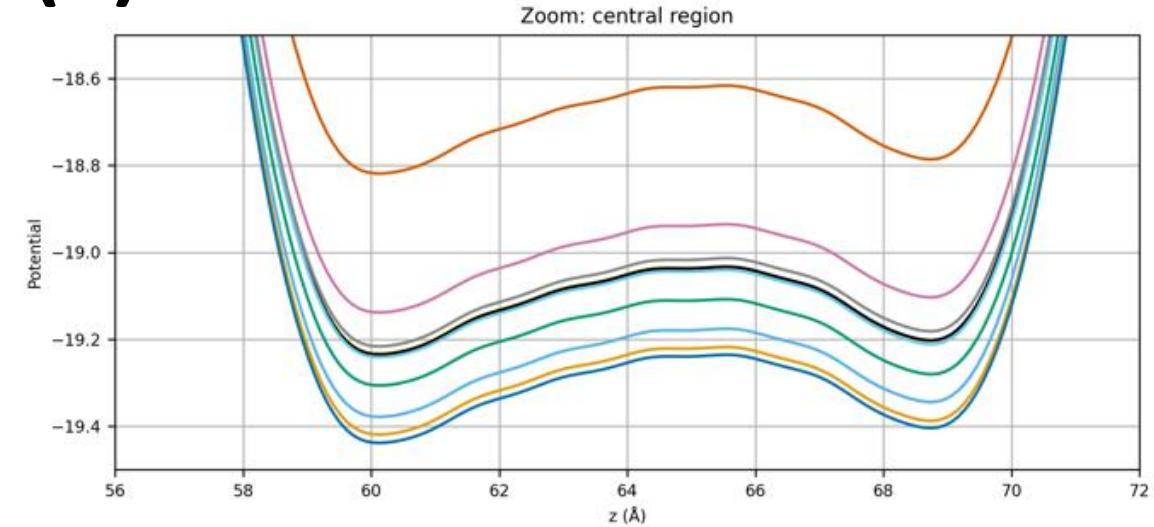
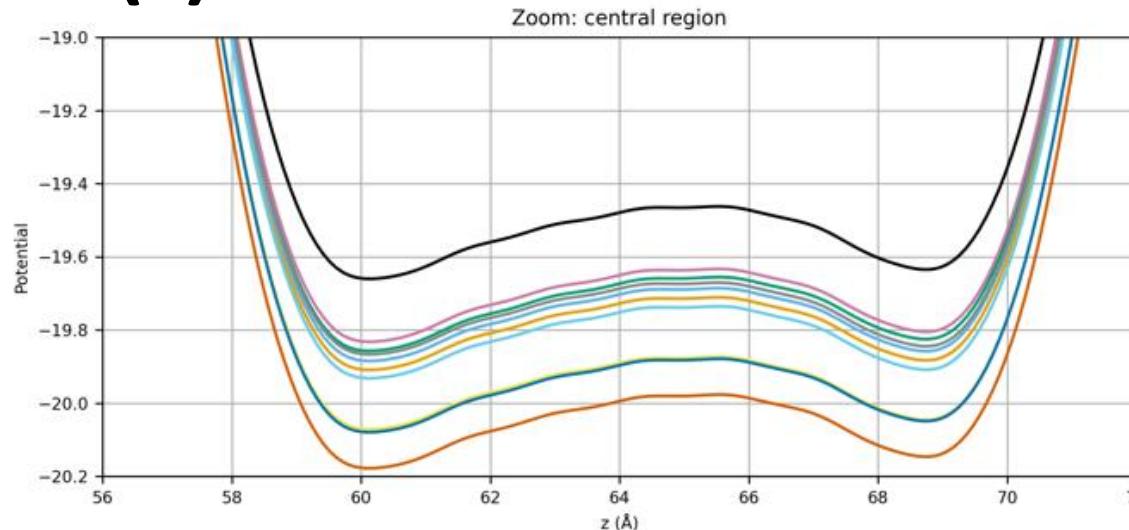
Zone di interesse



(a)**Nessun difetto****(b)****Difetto superficiale Si^+** **(C) Difetto superficiale O^-** 

- Shift 1
- Shift 2
- Shift 3
- Shift 4
- Shift 5
- Shift 6
- Shift 7
- Shift 8
- Shift 9
- Shift 10

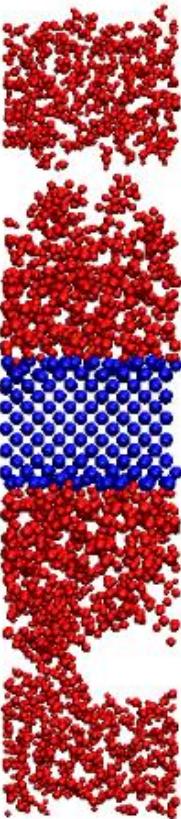


(a)**Nessun difetto superficiale****(b)****Difetto superficiale Si⁺****(c)****Difetto superficiale O⁻**

- Shift 1
- Shift 2
- Shift 3
- Shift 4
- Shift 5
- Shift 6
- Shift 7
- Shift 8
- Shift 9
- Shift 10

- Maggiore differenza di potenziale nel caso Si⁺ (**circa 0,6eV**).
- Spazio tra le bande

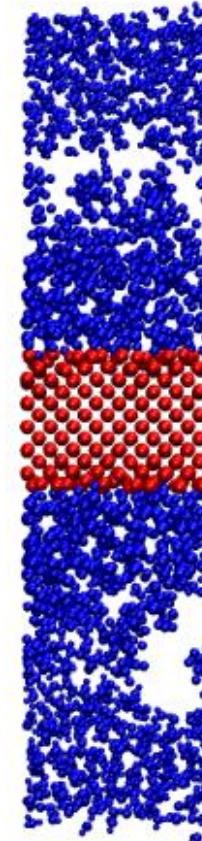
Analisi della carica di Bader



Carica esterna = carica H₂O + carica CAF + carica SiO₂

Carica interna = carica Si + carica B

Shift 10 – shift 1		
Difetto	Esterna	Interna
N.D	0,001	-0,001
Si ⁺	-0,09	0,09
O ⁻	0,02	-0,02

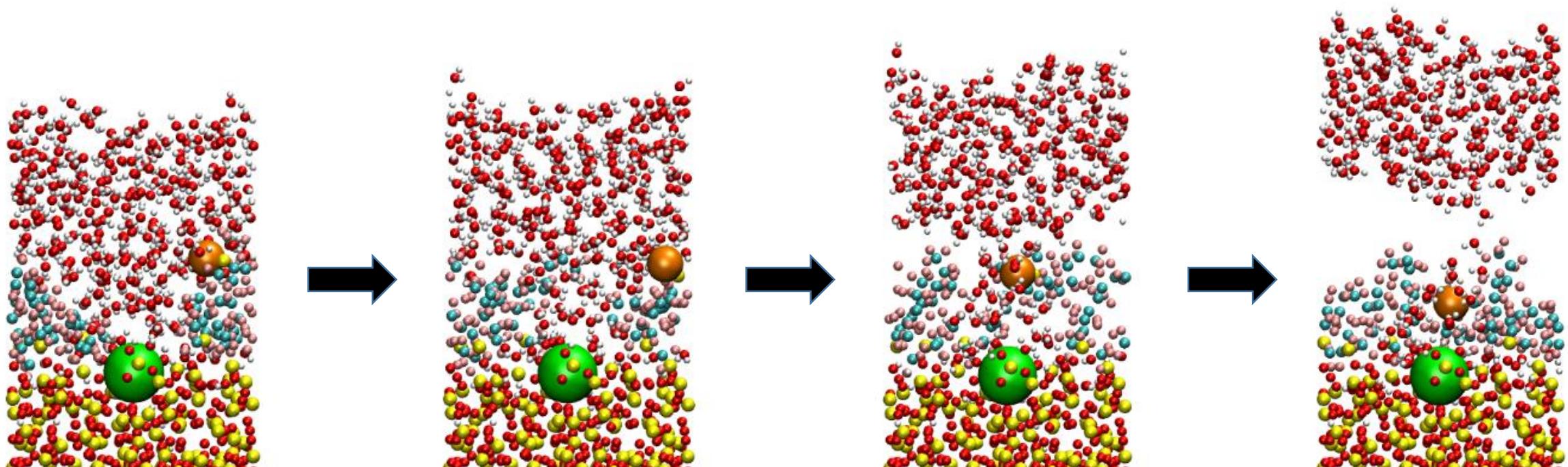


Carica negativa



Carica positiva

Ipotesi di meccanismo



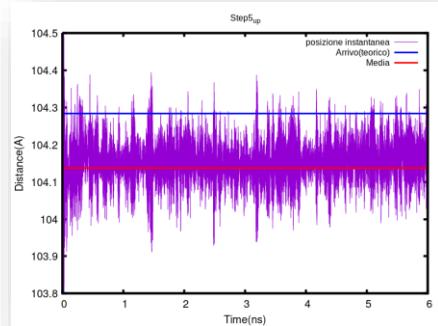
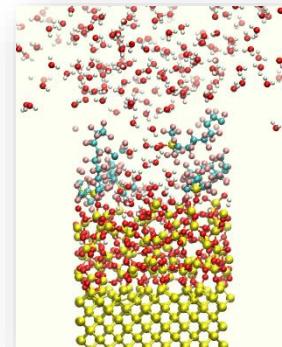
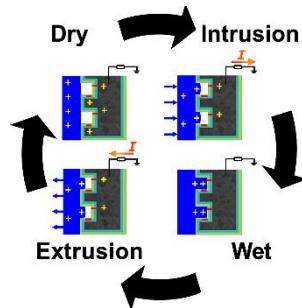
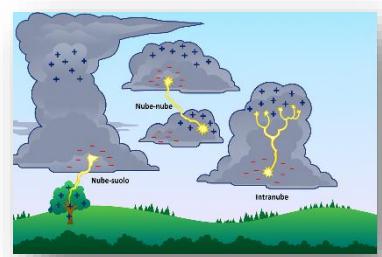
O⁻ localizzato sulla catena alchilica libera



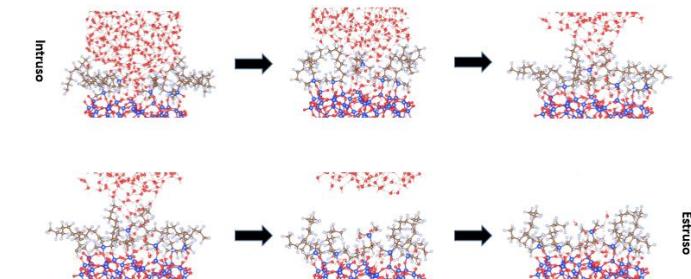
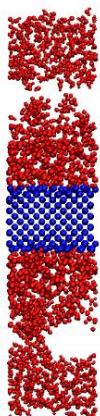
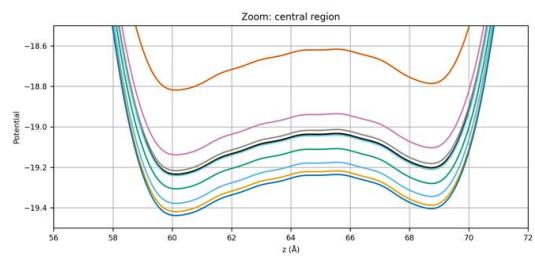
Difetto superficiale Si⁺

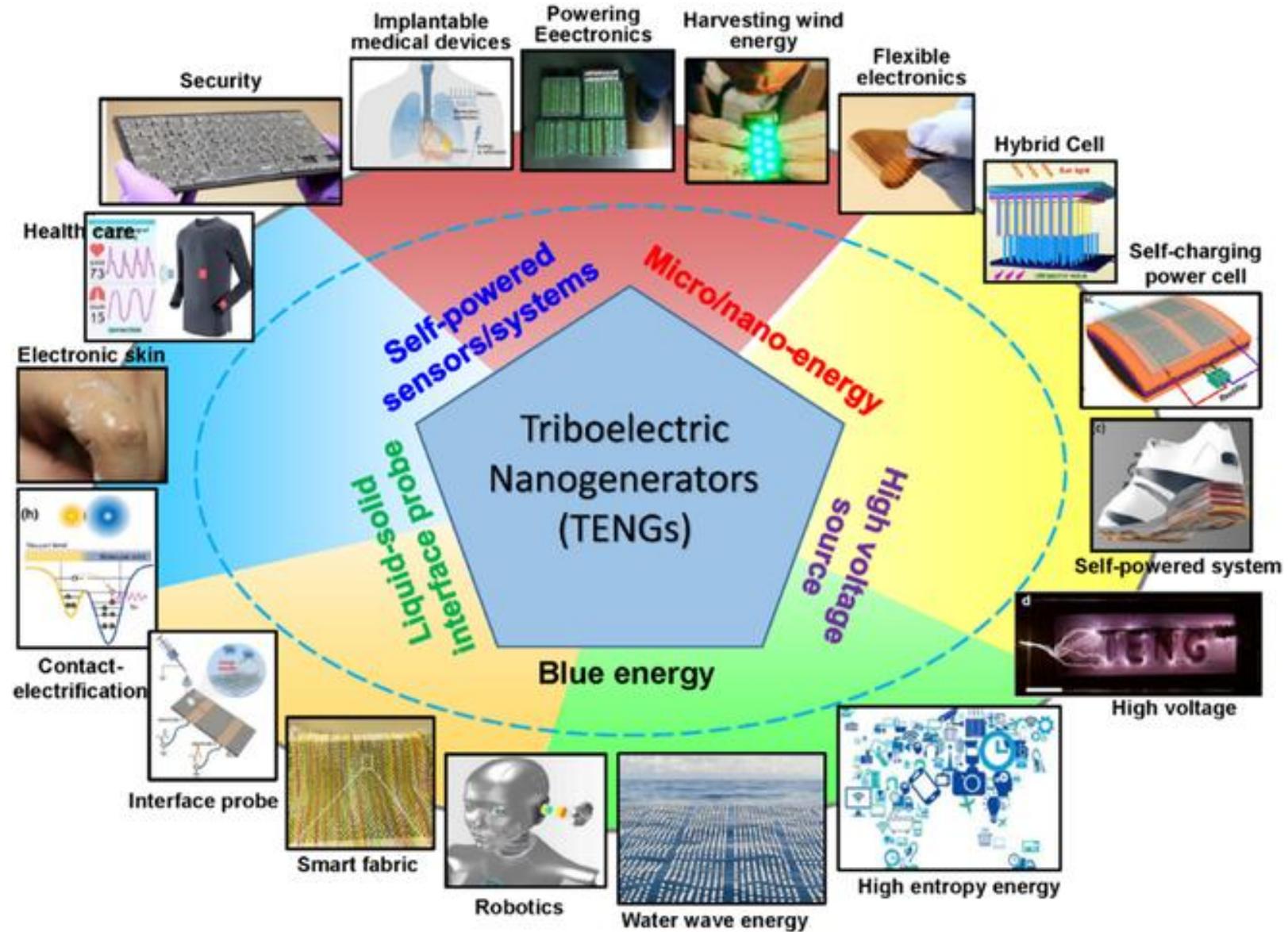
Conclusioni

- ❖ Il difetto superficiale di Si^+ porta una maggiore differenza di potenziale.
- ❖ In base al tipo di difetto creato è possibile stabilire il verso di circolazione della corrente.
- ❖ Abbiamo ipotizzato un meccanismo, da verificare con calcoli più accurati sulla densità elettronica.

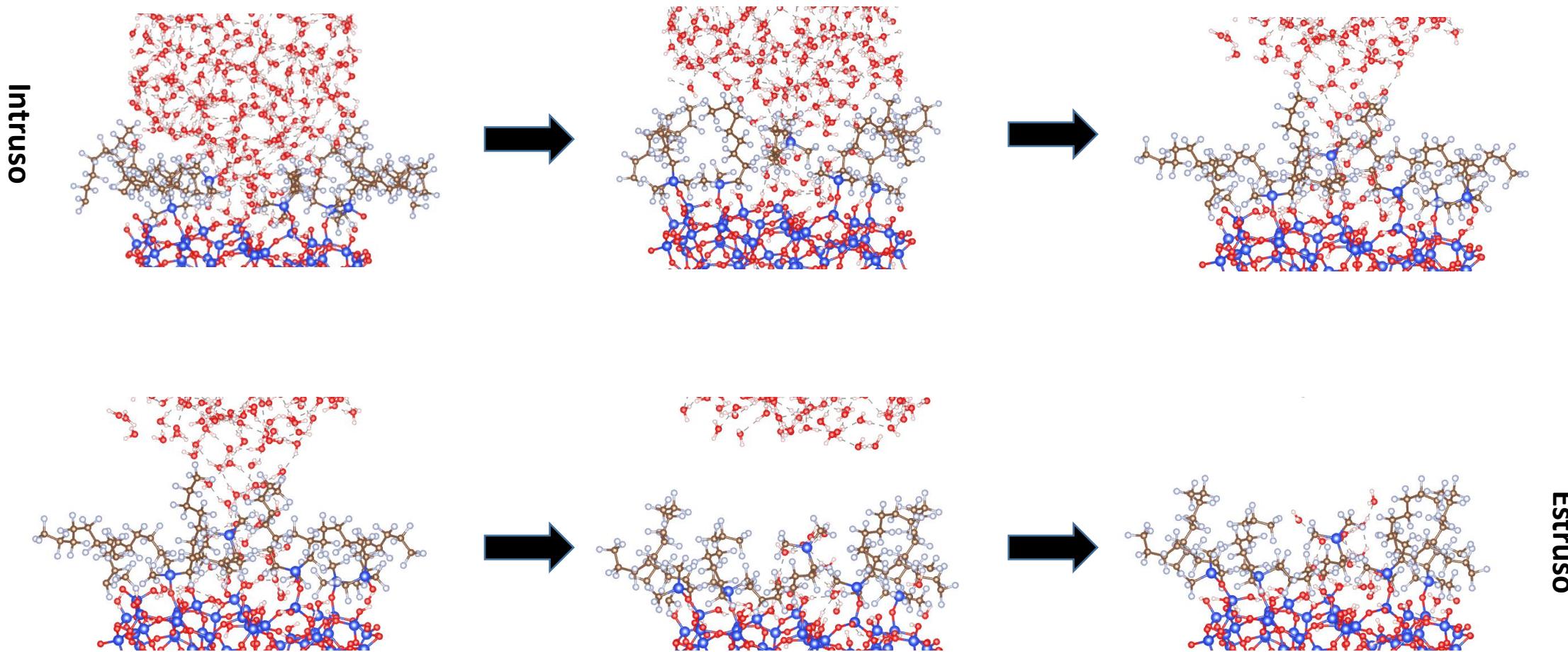


Grazie per l'attenzione





Meccanismo proposto



Analisi della carica di Bader

- Un ulteriore aspetto preso in analisi riguarda come la carica si distribuisca nel sistema durante i vari shift.
- L'analisi, condotta tramite l'algoritmo di Bader, ha permesso di suddividere la densità elettronica tra le diverse specie atomiche, attribuendo così a ogni atomo un numero definito di elettroni.
- I contributi relativi agli atomi appartenenti a uno stesso layer del sistema sono stati sommati, così da ottenere il numero effettivo di elettroni presenti nelle diverse regioni.
- carica netta (e) = elettroni di valenza nominali - elettroni trovati (da Bader)
- Le unità sono sempre in e (carica elementare), e un numero positivo indica una perdita di densità elettronica (atomo positivo), negativo un guadagno.

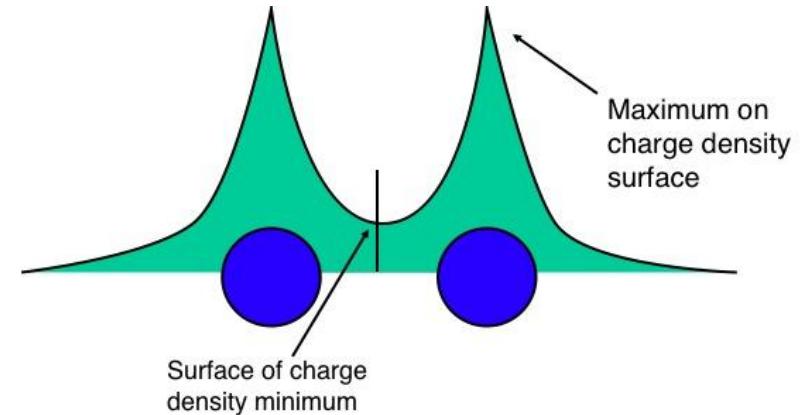


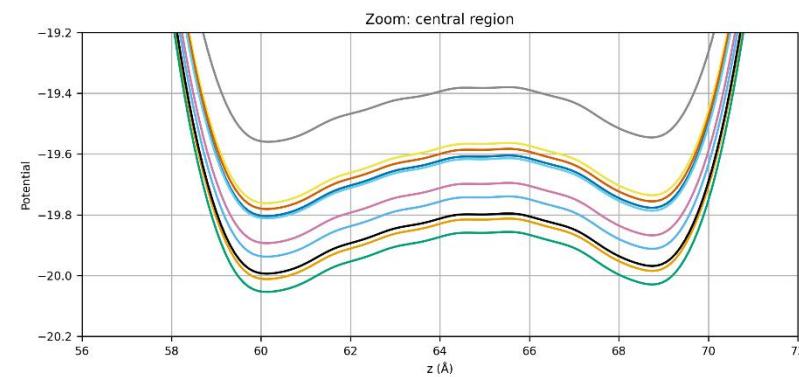
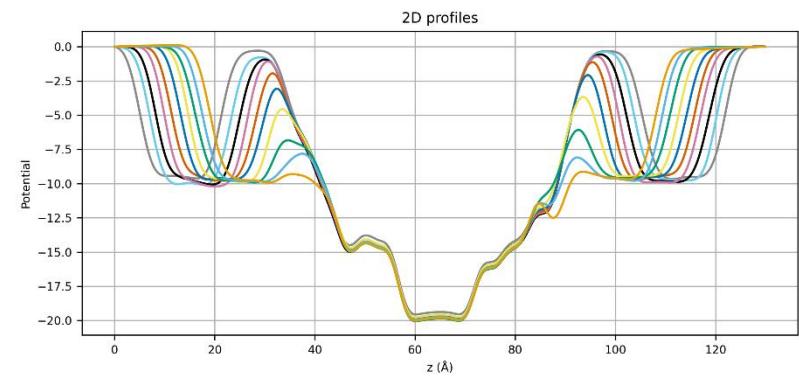
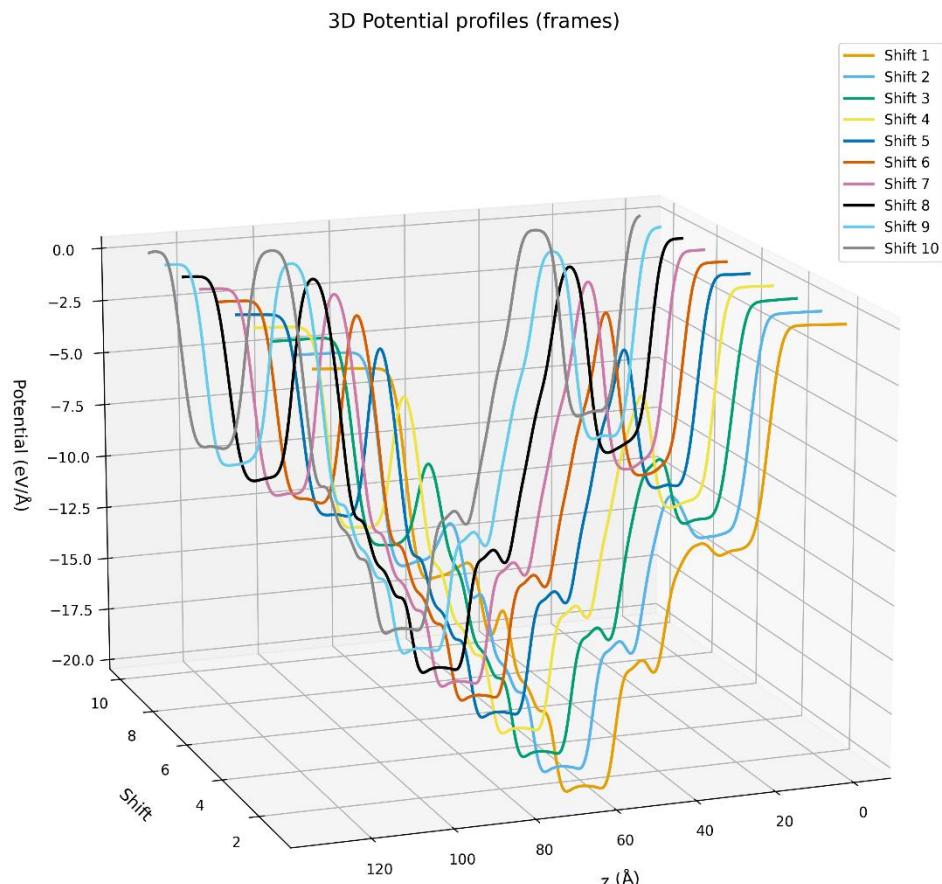
Tabella di carica Si⁺

Shift	C.A.F	Silice	H2O	Silicio	B
1	-31.095	-35.426	0.663	66.325	-0.467
2	-30.947	-35.330	0.389	66.355	-0.467
3	-30.855	-35.235	0.329	66.227	-0.467
4	-30.721	-35.387	0.272	66.303	-0.467
5	-30.686	-35.370	0.147	66.377	-0.468
6	-30.690	-35.270	0.132	66.294	-0.467
7	-30.608	-35.451	0.115	66.411	-0.467
8	-30.684	-35.434	0.185	66.400	-0.467
9	-30.646	-35.556	0.343	66.326	-0.467
10	-30.612	-35.567	0.226	66.419	-0.466
Diff(10-1)	0.483	-0.140	-0.437	0.093	0.001

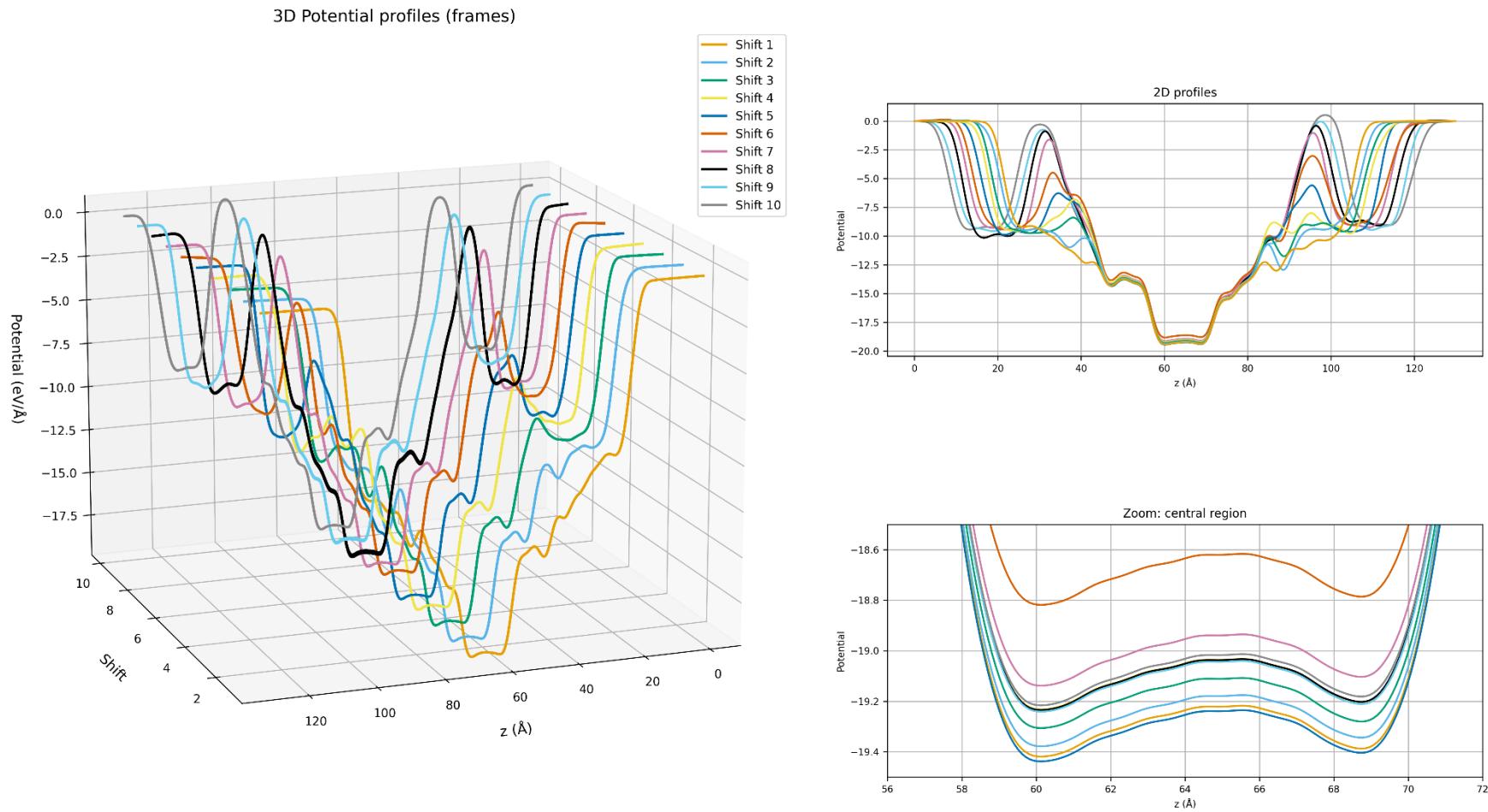
Tabella di carica O⁻

Shift	C.A.F	Silice	H2O	Silicio	B
1	-31.305	-35.097	0.585	66.284	-0.467
2	-31.124	-35.092	0.440	66.243	-0.467
3	-31.122	-35.096	0.365	66.320	-0.467
4	-31.107	-35.064	0.358	66.280	-0.467
5	-30.920	-35.219	0.267	66.339	-0.467
6	-30.977	-35.079	0.195	66.328	-0.467
7	-30.870	-35.115	0.204	66.248	-0.467
8	-30.893	-35.244	0.325	66.280	-0.467
9	-30.881	-35.259	0.355	66.252	-0.467
10	-30.962	-35.295	0.460	66.263	-0.467
Diff(10-1)	0.343	-0.197	-0.124	-0.021	-0.000

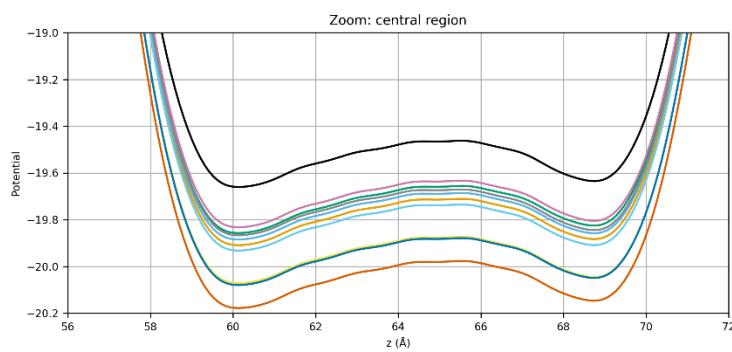
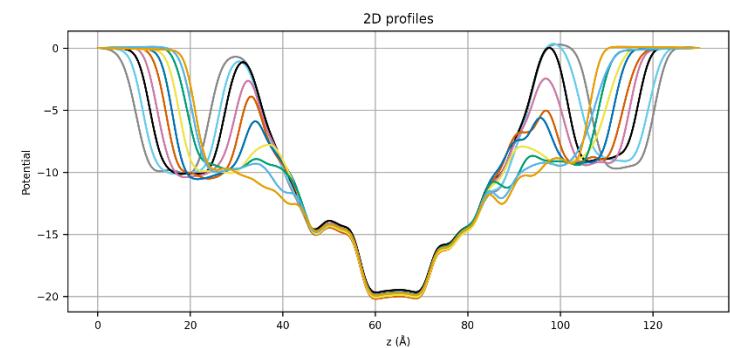
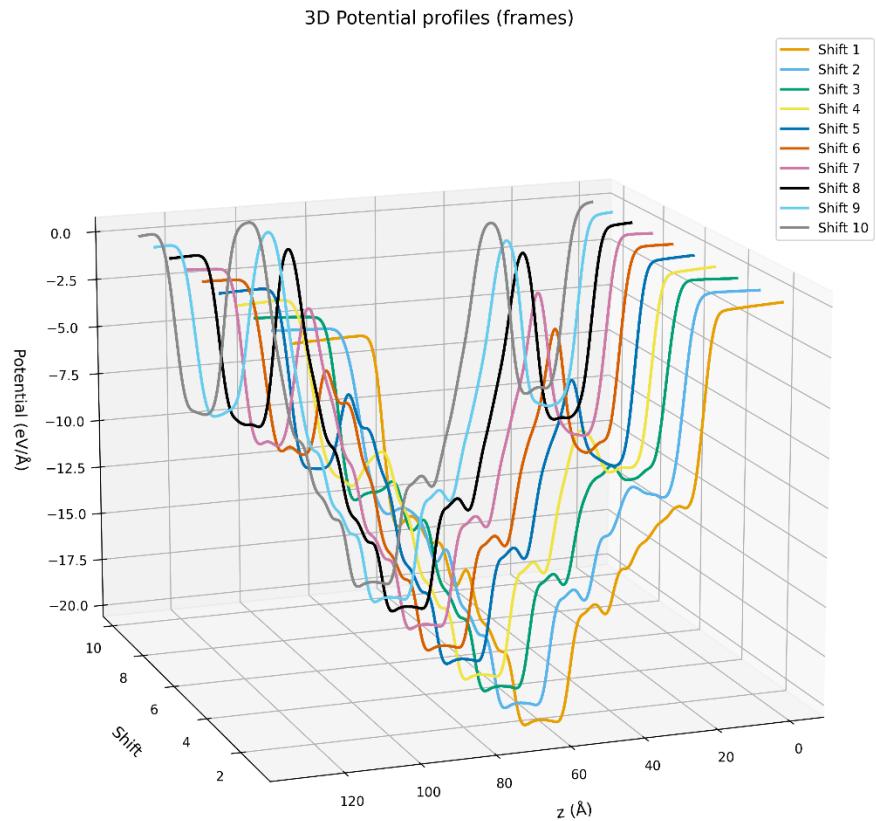
Clean



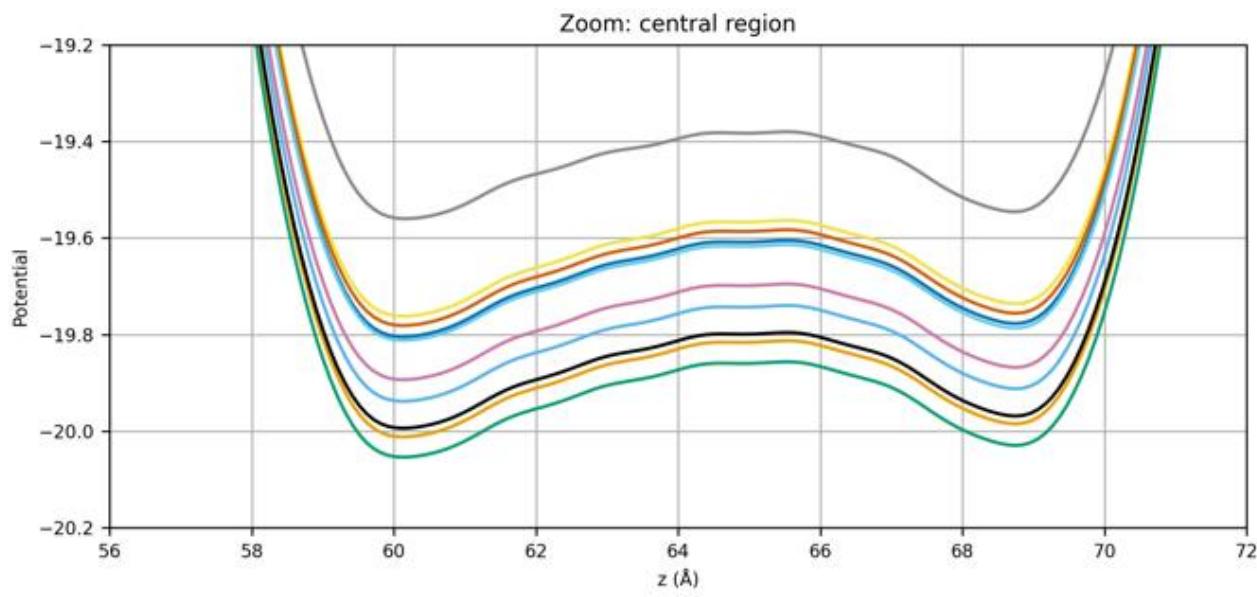
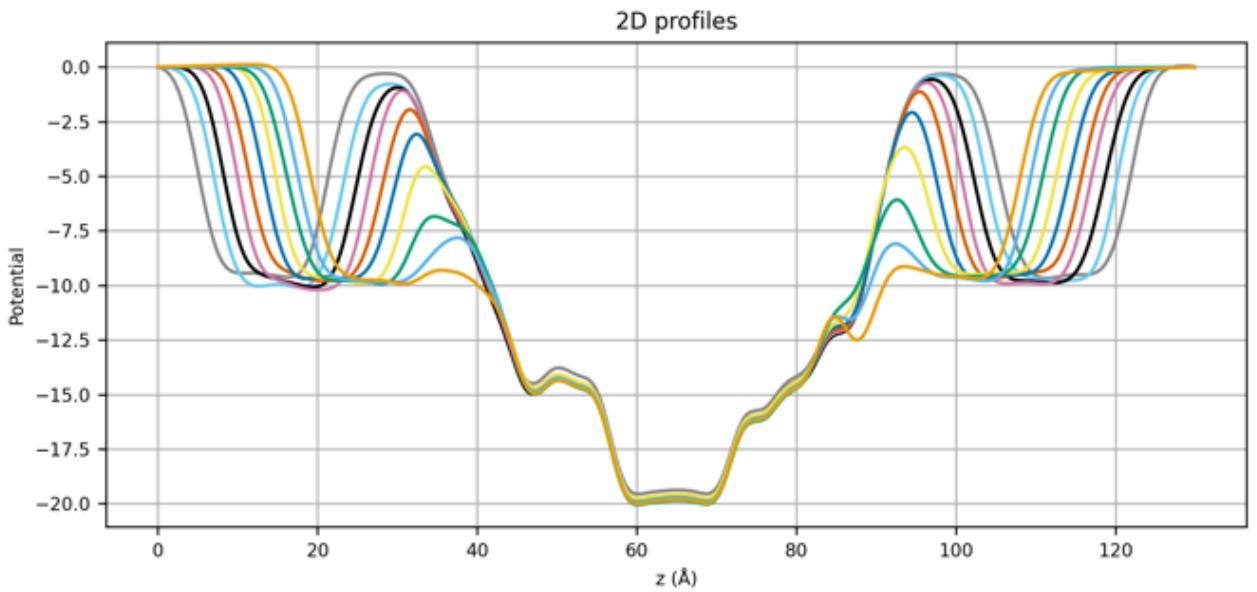
Si



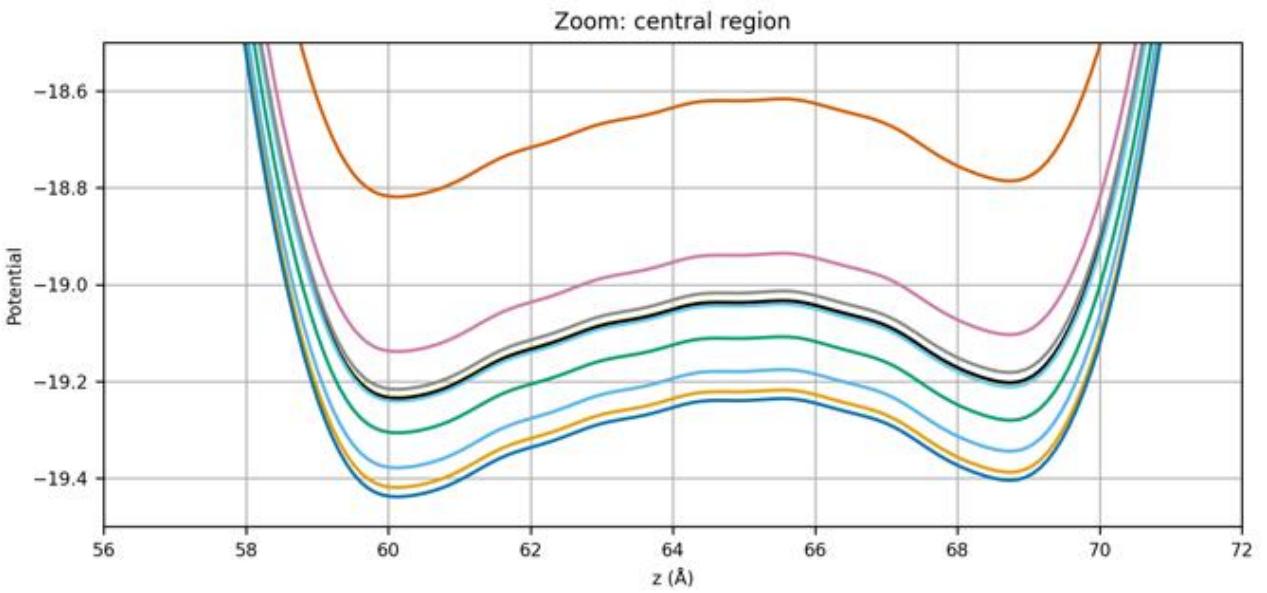
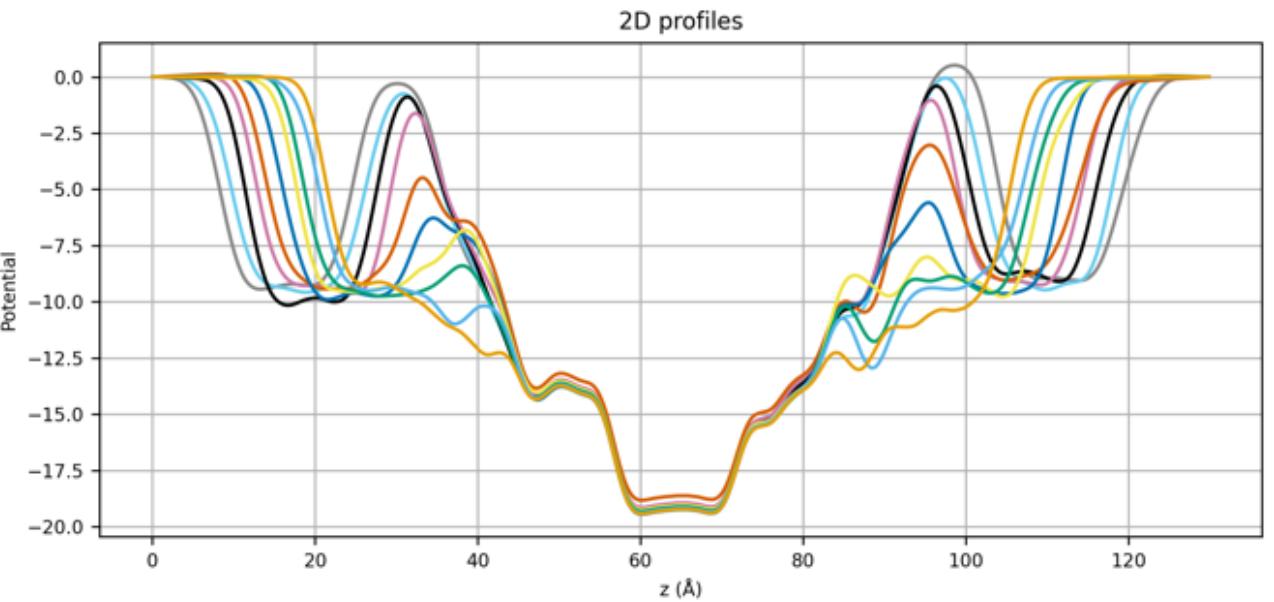
O



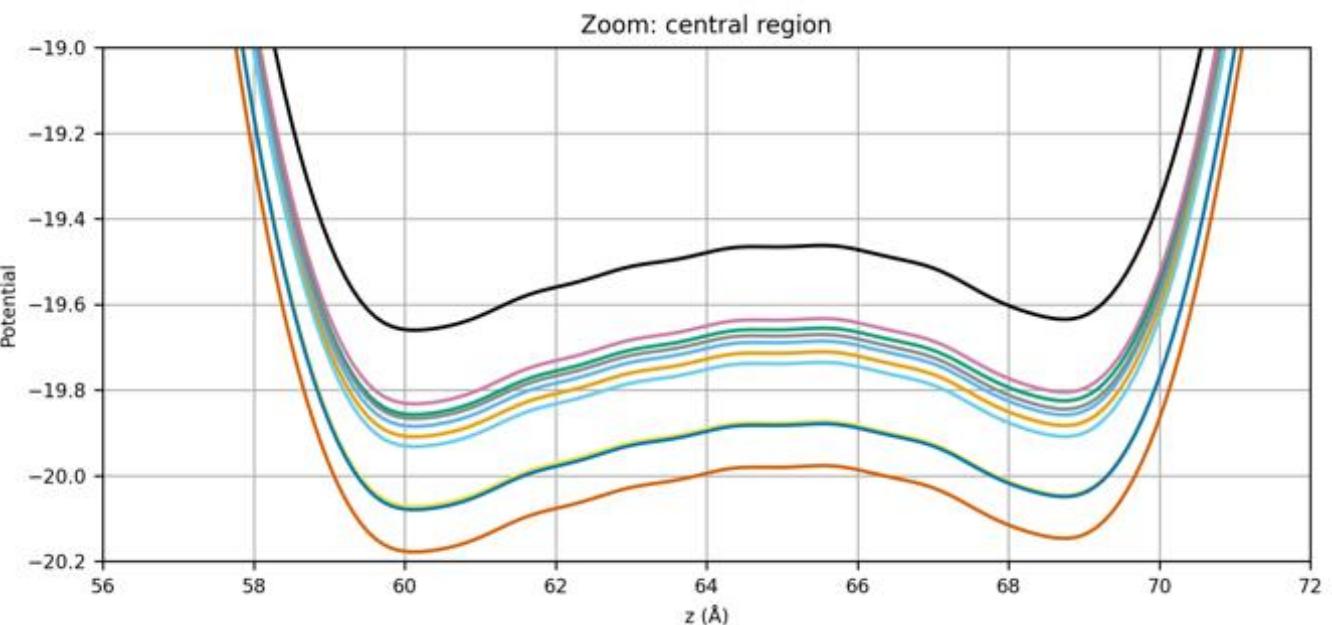
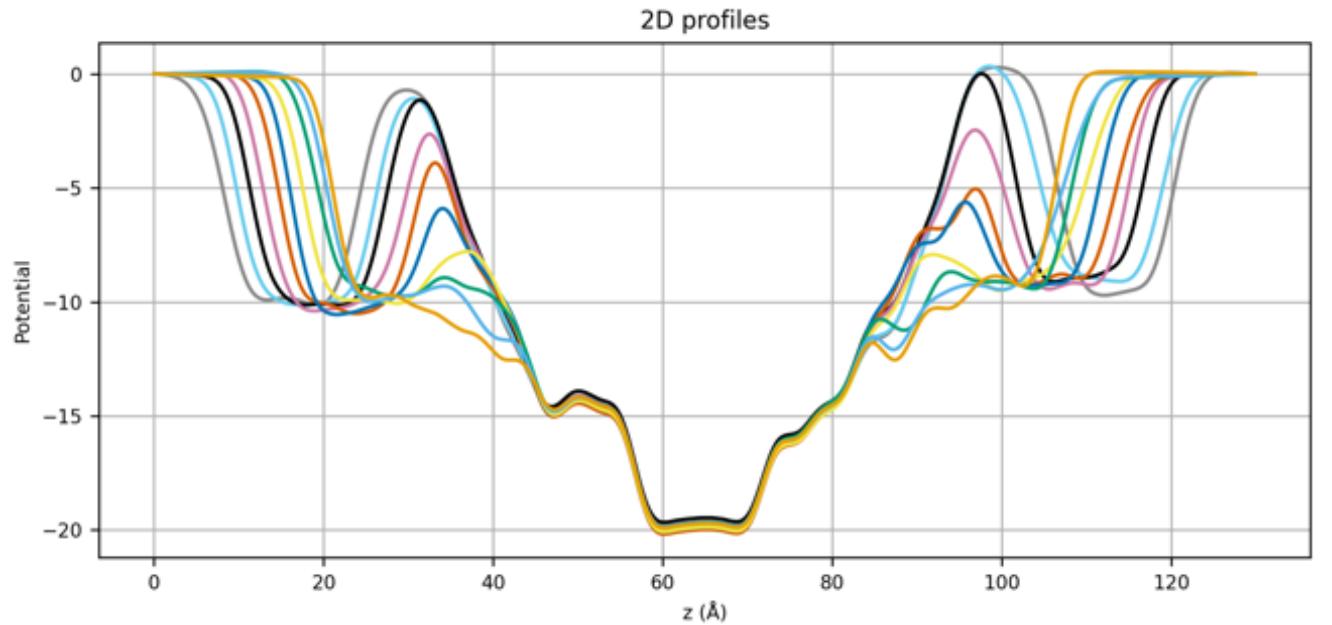
Nessuna carica



$\text{Si}^+ e^- [\text{C}_8 - \text{CF}_{30}]^-$



$O^- e^- [C_8 - CF_3Si]^+$



Distanza tra O e Si (cariche)

