Summer school
Physical Sensing and Processing

Intro to Molecular dynamics

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What is Molecular Dynamics

Molecular Dynamics (MD) allows to study the evolution of atoms and molecules over a certain period of time. The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles

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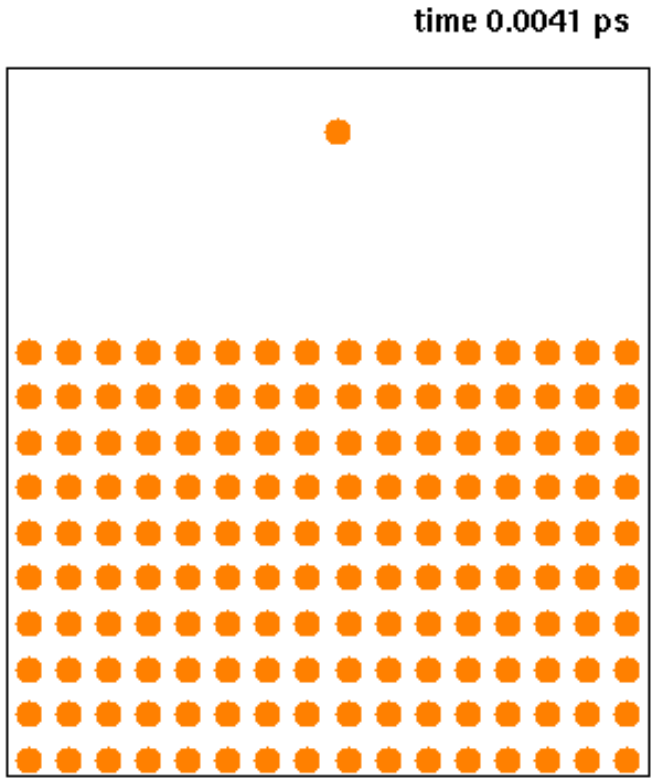

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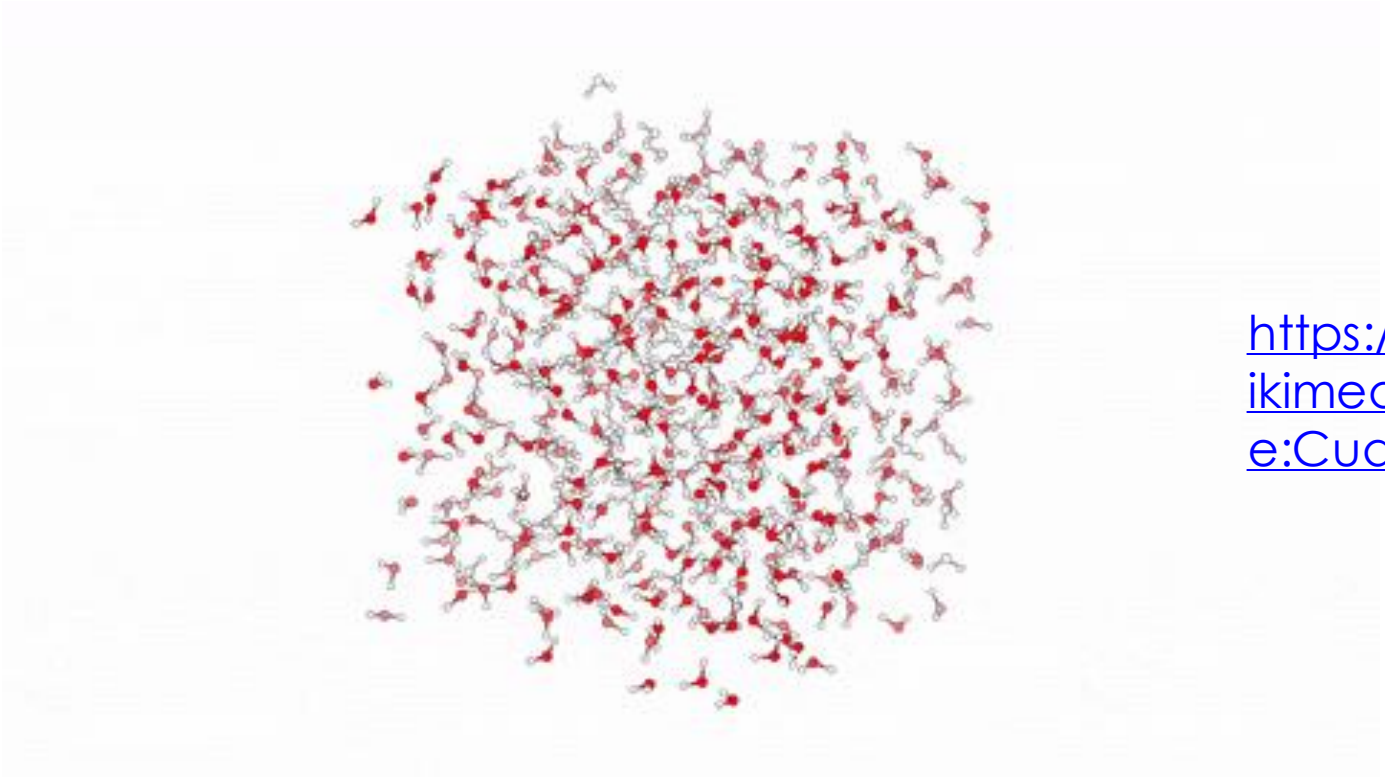

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The large number of particles in the systems does not allow to determine physical properties analytically. We need to apply statistical approaches (e.g., computing averages) to get the thermodynamics properties of the system

Different types of MD

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We can talk about:

- Classical MD (where the interatomic potential derives from analytical force fields)
- *Ab initio* MD (where the interatomic potential derives from first-principles calculations)
- Machine-learning-based MD (where the interatomic potential can be obtained from a machine learning algorithm)
- Hybrid MD (where it is possible to mix different approaches)

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Regardless these different methods, the foundation of MD relies on solving the Newton's equations of motion

Evolving MD simulations

MD consists in the numerical solution of the equations of motion

$$m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{f}_i \qquad \boldsymbol{f}_i = -\frac{\partial}{\partial \boldsymbol{r}_i}\mathcal{U}$$

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The main point in MD is finding a certain form of the interatomic forces (also known as force fields) to solve the differential equation on the left.

MD simulations: the actual algorithm

Once you compute the force field, how do you evolve the system? You need to solve the Newton's equations. You can do that by applying several types of integrators:

- Verlet algorithm
- Leap-Frog
- Velocity Verlet
- Beeman's Method
- Gear Method

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MD simulations: Velocity Verlet algorithm

Within the different numerical integrators, Velocity Verlet is the most used in MD codes. The basic structure of the algorithm is the following

$$\boldsymbol{p}_i(t+\tfrac{1}{2}\delta t) = \boldsymbol{p}_i(t) + \tfrac{1}{2}\delta t \boldsymbol{f}_i(t)$$
$$\boldsymbol{r}_i(t+\delta t) = \boldsymbol{r}_i(t) + \delta t \boldsymbol{p}_i(t+\tfrac{1}{2}\delta t)/m_i$$
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Advantages:

- it is time reversible
- It is symplectic (i.e., the volume in phase space is conserved)
- it is low order in time, allowing long timesteps
- it is easy to program and requires less memory

MD simulations: workflow

Using one of the algorithm to solve the Newton's equations and having a specific force fields allows to run the MD workflow

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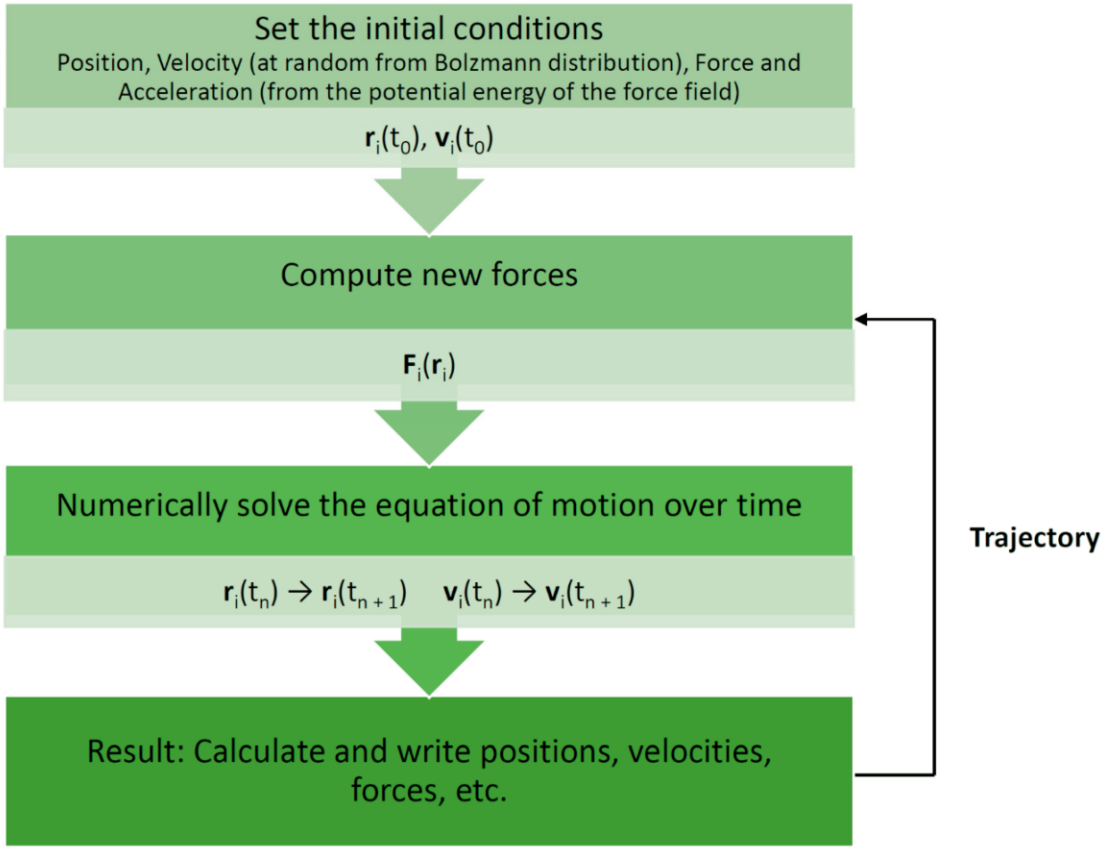
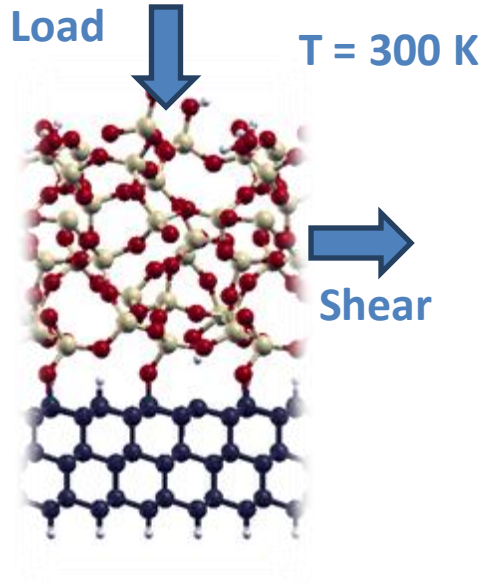


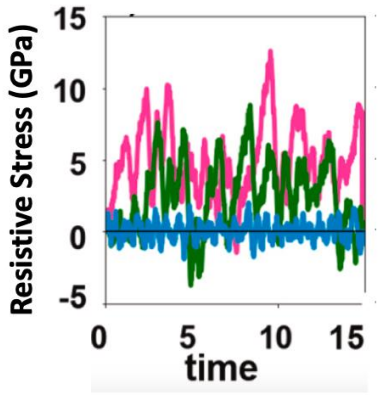
Processes **9**, 71 (2021)

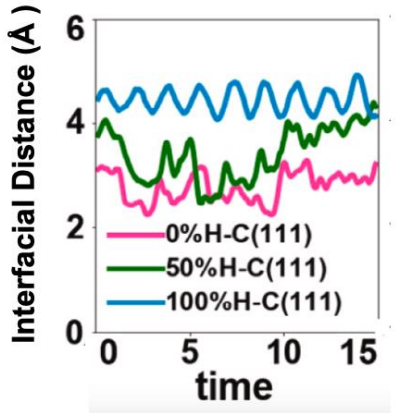
System of interest: Silica-Diamond interface

- First principles calculations based on density functional theory (DFT) → high accuracy (and high computational cost)

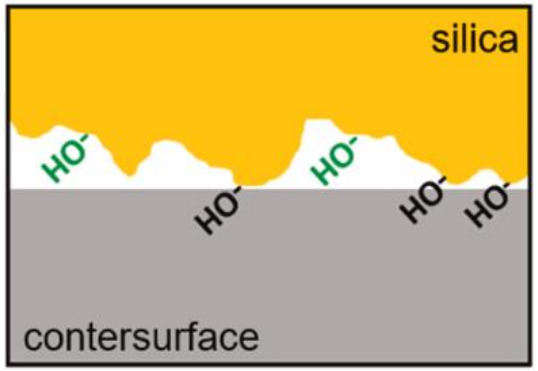
- *Ab initio* molecular dynamics (MD) → simulate sliding interfaces

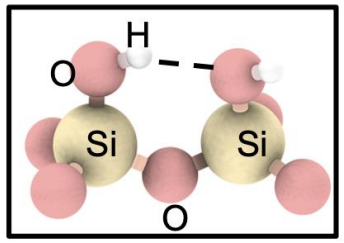




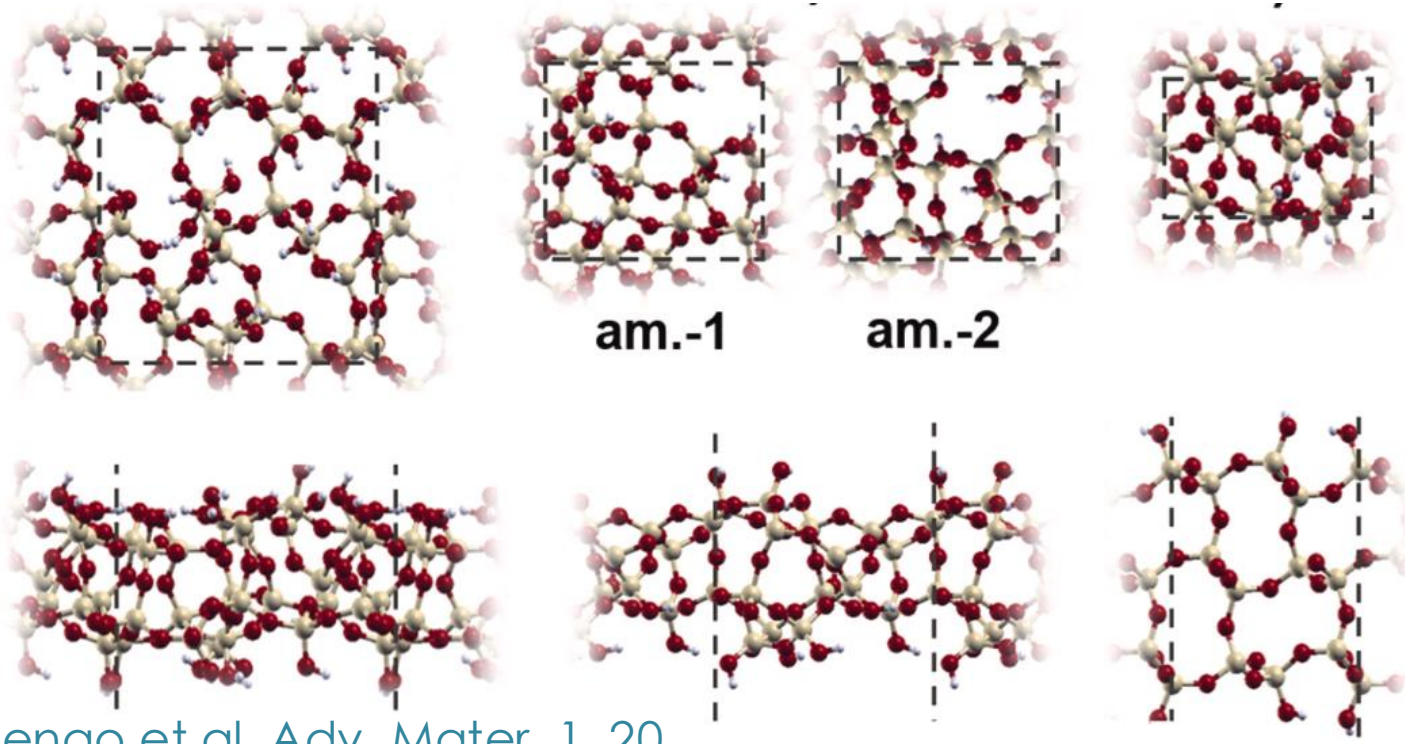


Amorphous SiO_2





Reference model | Present models | Cristobalite (101)

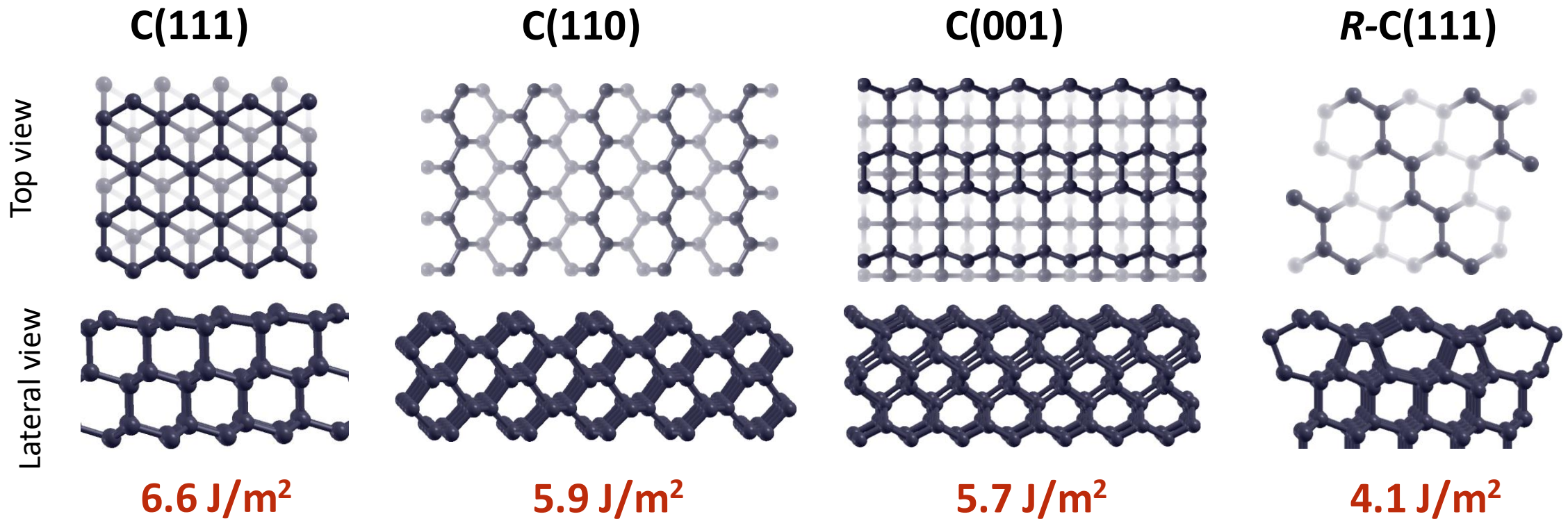


P. Ugliengo et al. Adv. Mater. 1, 20 (2008)

	Smaller model				Large reference model			
	MEAN	**SD**	**MAX**	**MIN**	MEAN	SD	MAX	MIN
lenght (Si-O) [Å]	**1.637**	**0.015**	**1.673**	**1.612**	1.638	0.014	1.677	1.609
Angle (Si-O-Si) [°]	**142.6**	**15.0**	**173.6**	**117.5**	144.6	11.2	168.5	129.0
Lenght (O-H) [Å]	**0.981**	**0.008**	**0.998**	**0.974**	0.982	0.009	1.000	0.972
lenght H-bond [Å]	**1.745**	**0.205**	**1.964**	**1.559**	1.893	0.156	2.085	1.655

	SiOSi (°)	n.SiOH inner	n.SiOH exposed	ρ – SiOH (nm^{-2})	A (nm^2)
Amorphous from Ref. [44]	144 ± 11	2	6	4.8	1.60
Cristobalite (101)	146 ± 4	0	2	4.6	0.76
Amorphous-1 (this work)	141 ± 15	1	2	3.4	0.89
Amorphous-2 (this work)	141 ± 15	3	2	5.6	0.89

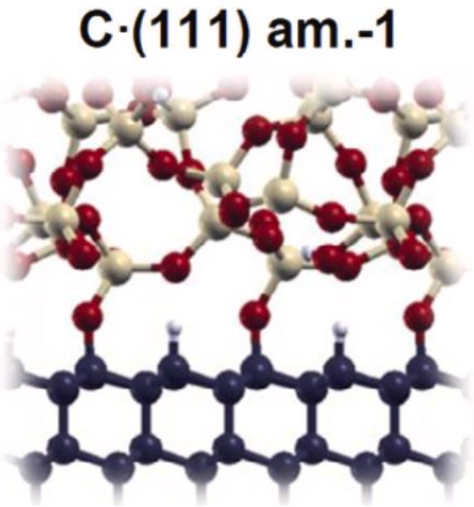
Low-indexes surfaces of diamond



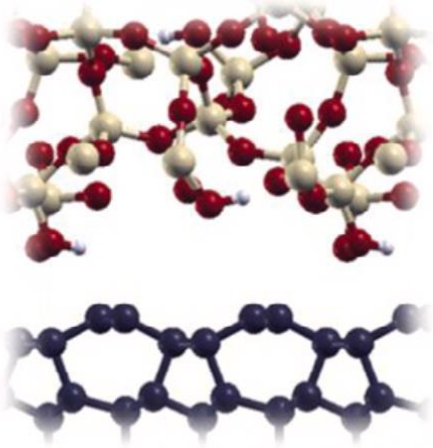
Surface energies by DFT-LDA

A. A. Stekolnikov, J. Furthmu¨ller, and F. Bechstedt, Phys. Rev B, 65, 115318 (2002)

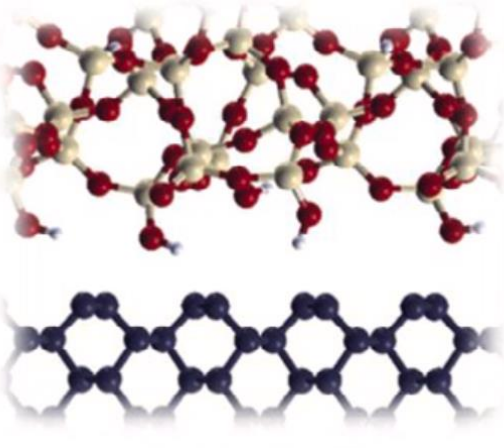
Effects of diamond orientation



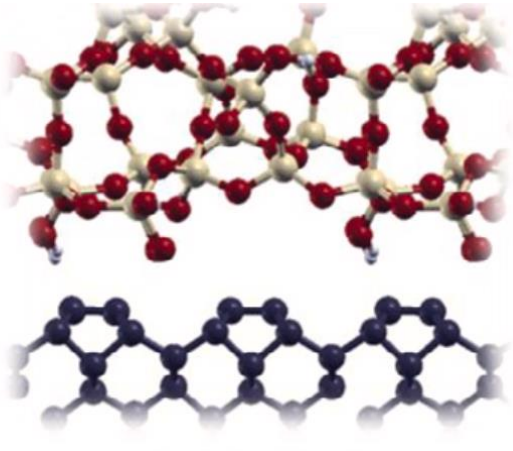
C(111)



R-C(111)



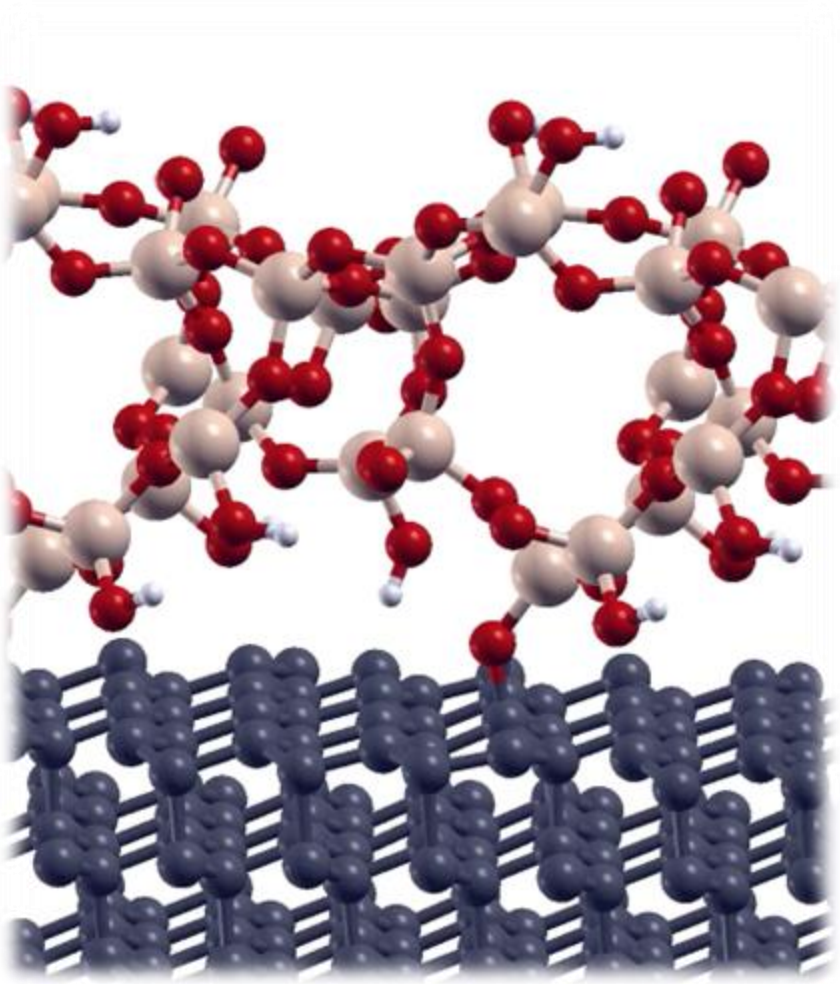
C(110)



C(001)

Optimized interfaces under 1 GPa load

Effects of diamond orientation



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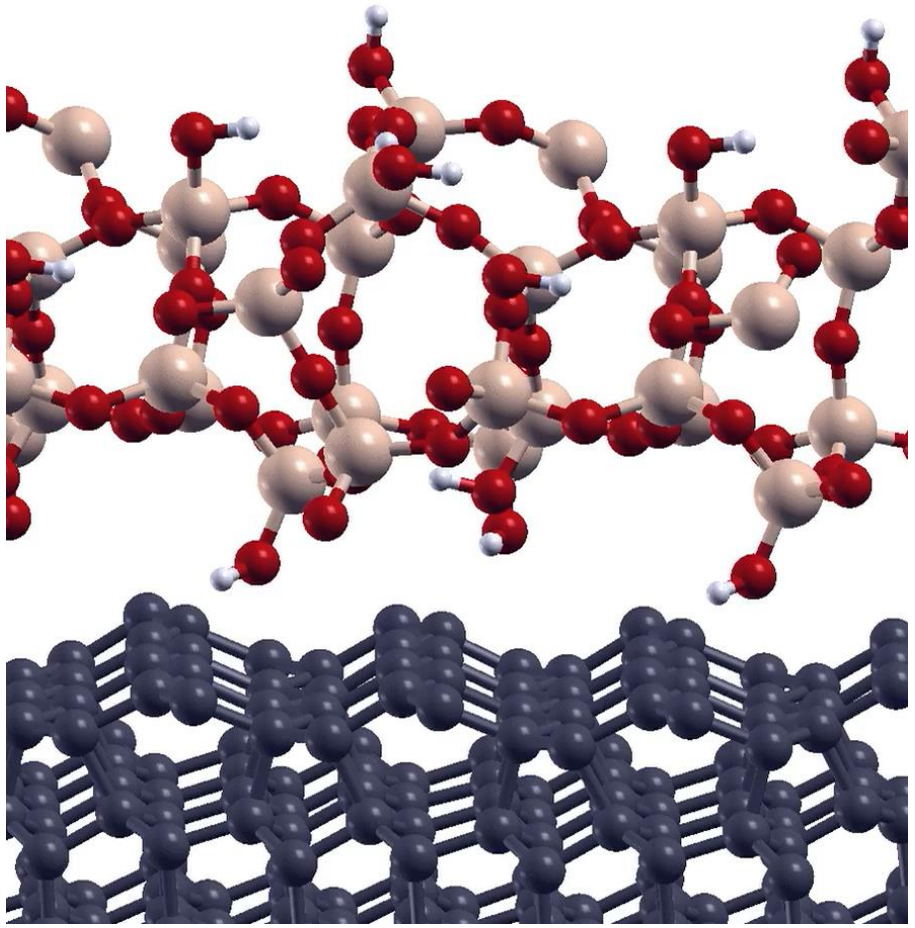

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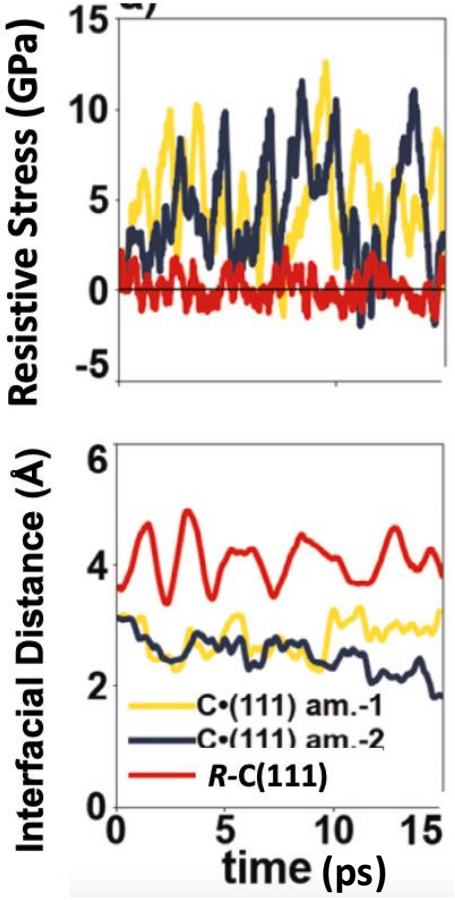
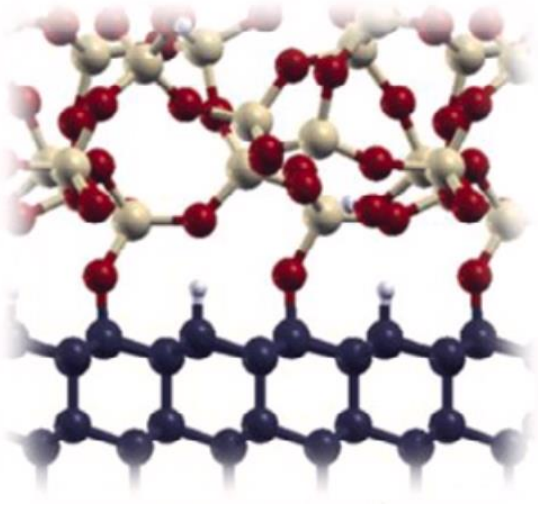
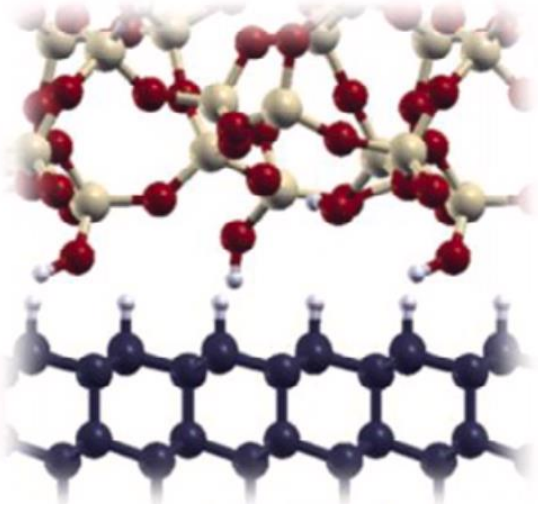


Effects of H-orientation

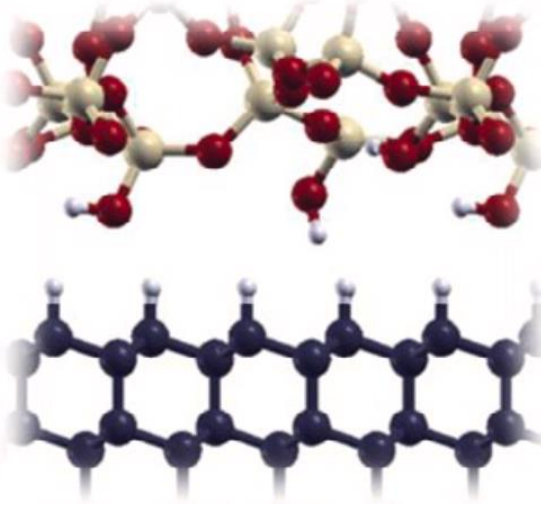
C·(111)



50%H-C(111)

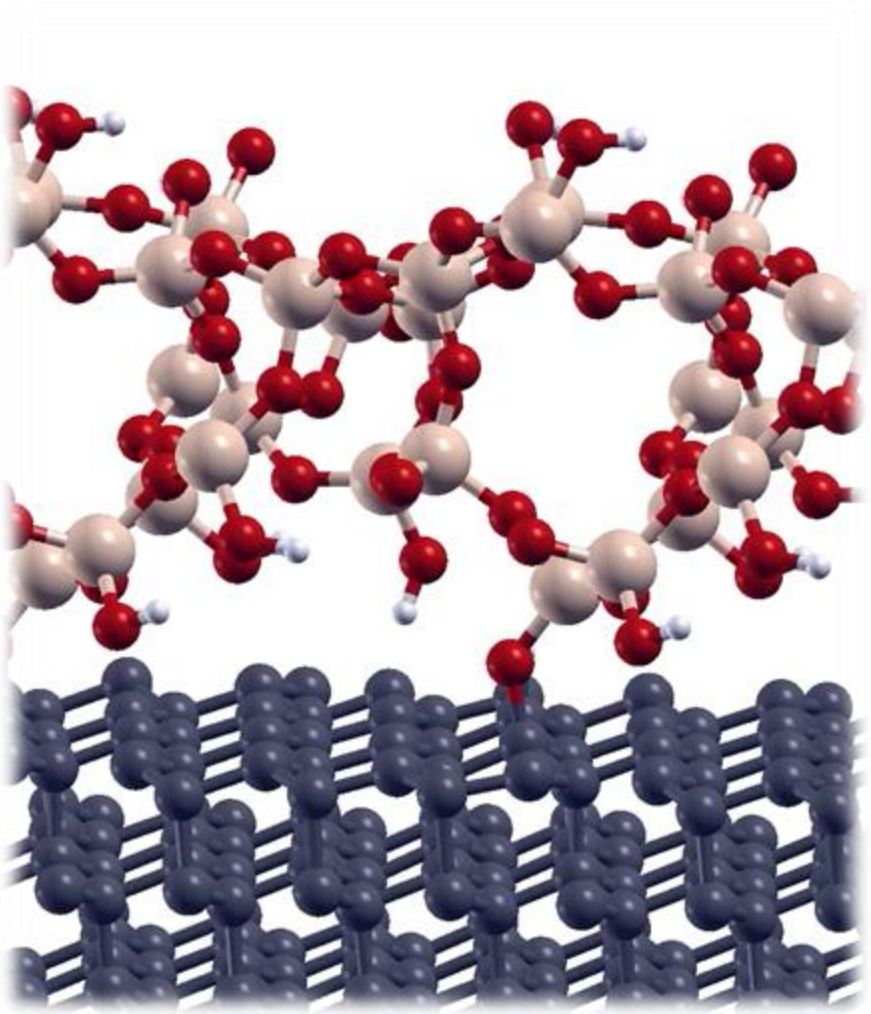


100%H-C(111)



Optimized interfaces at 1 GPa load

Effects of H-orientation



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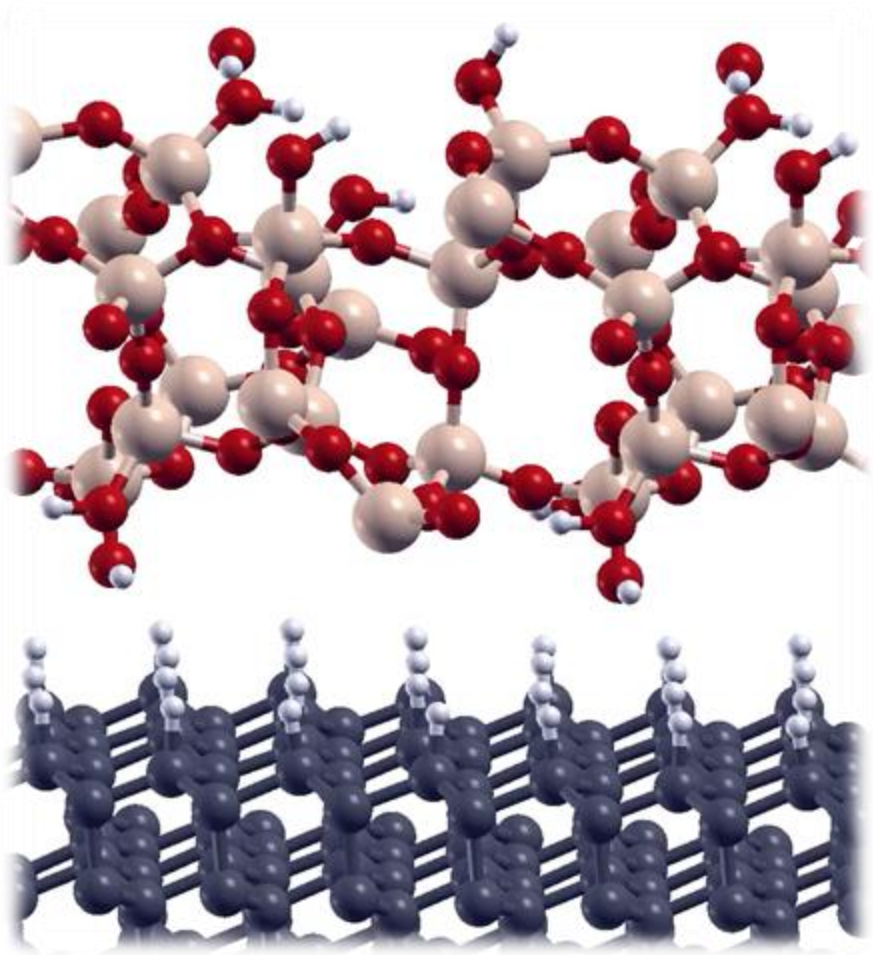

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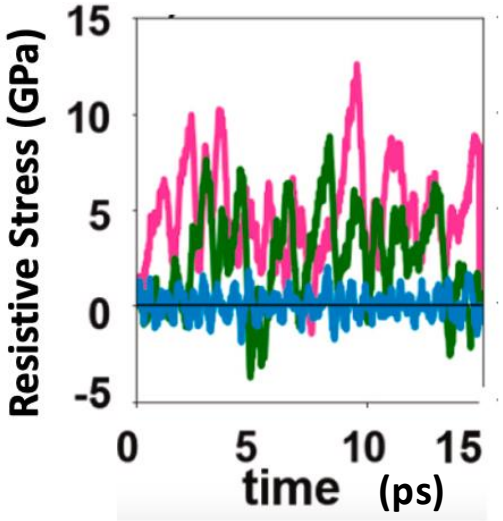
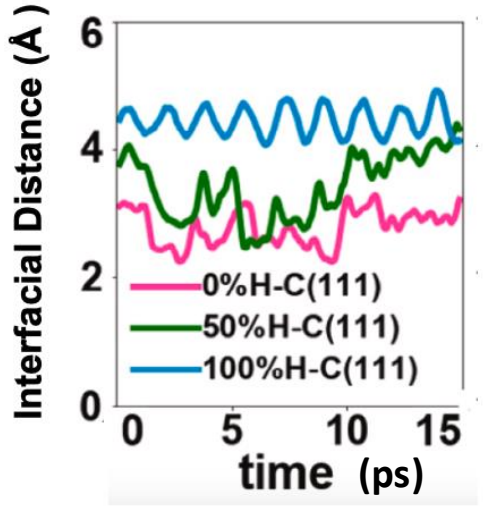
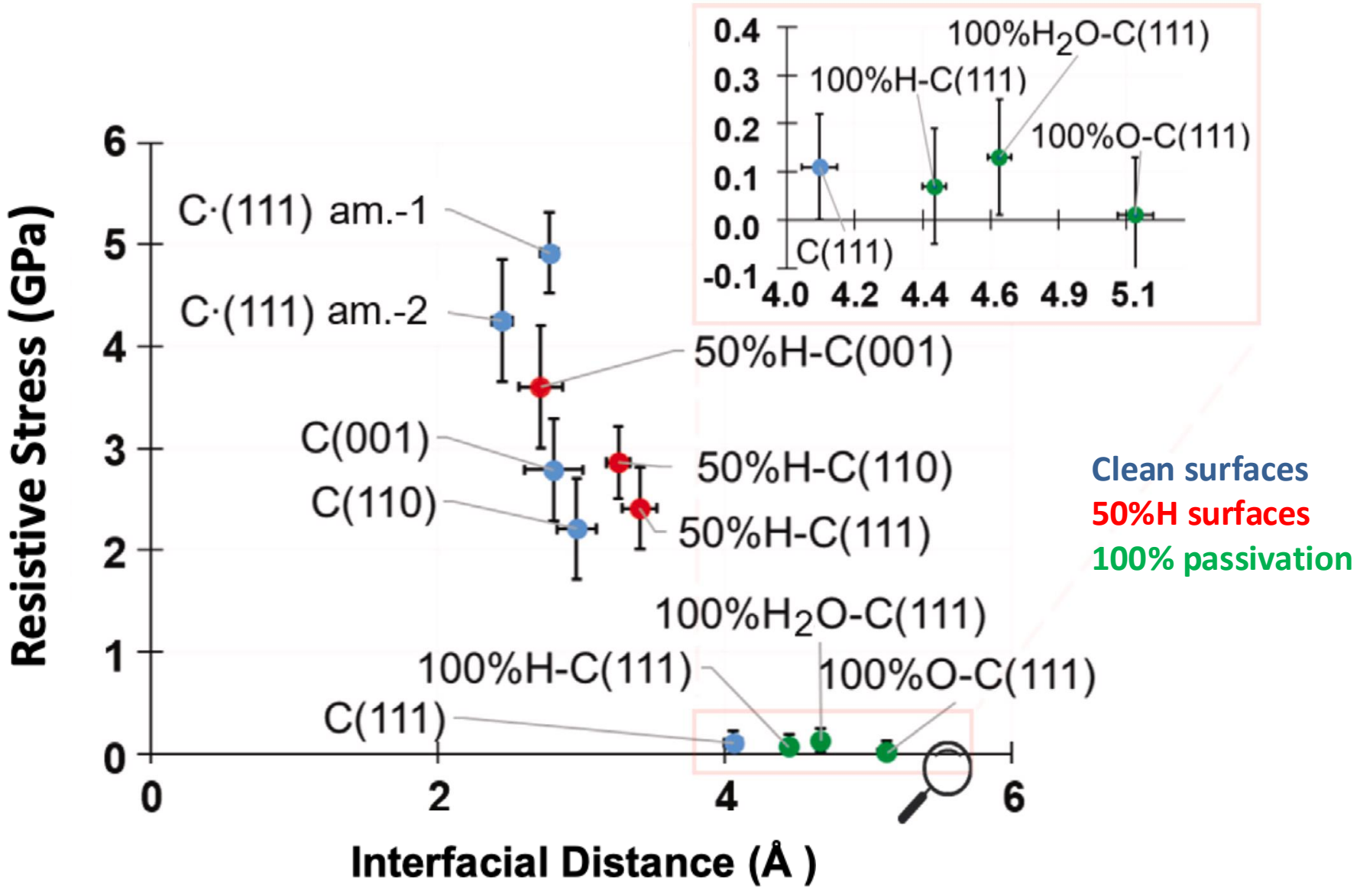
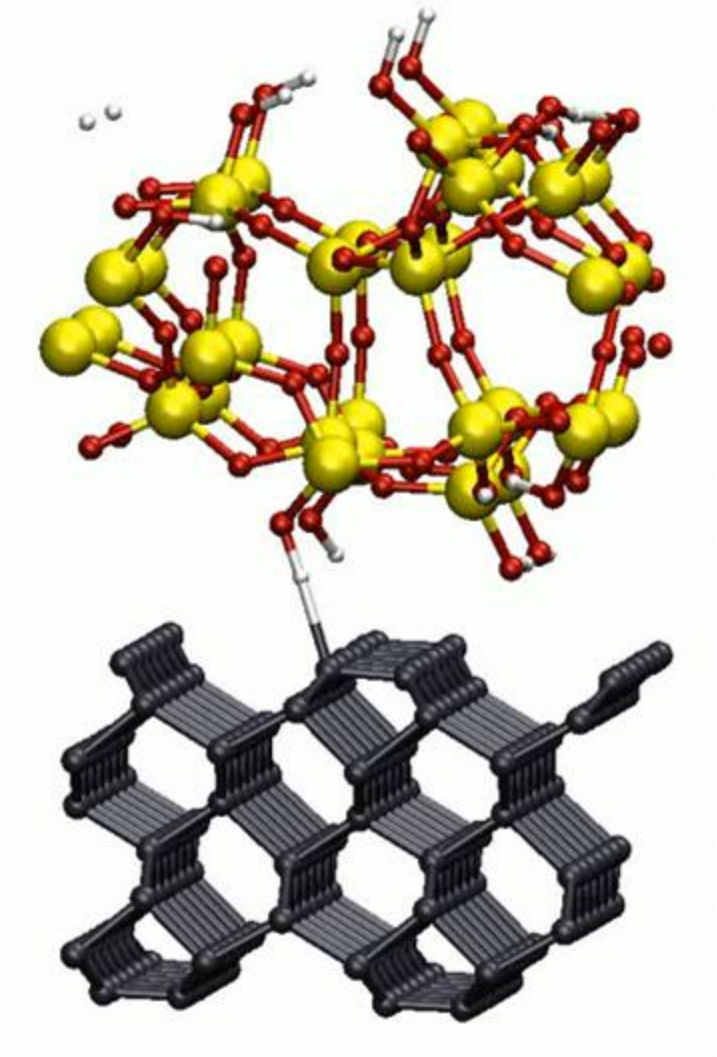




Average values



System of interest: Silica-Diamond interface



Silica-C(001) clean

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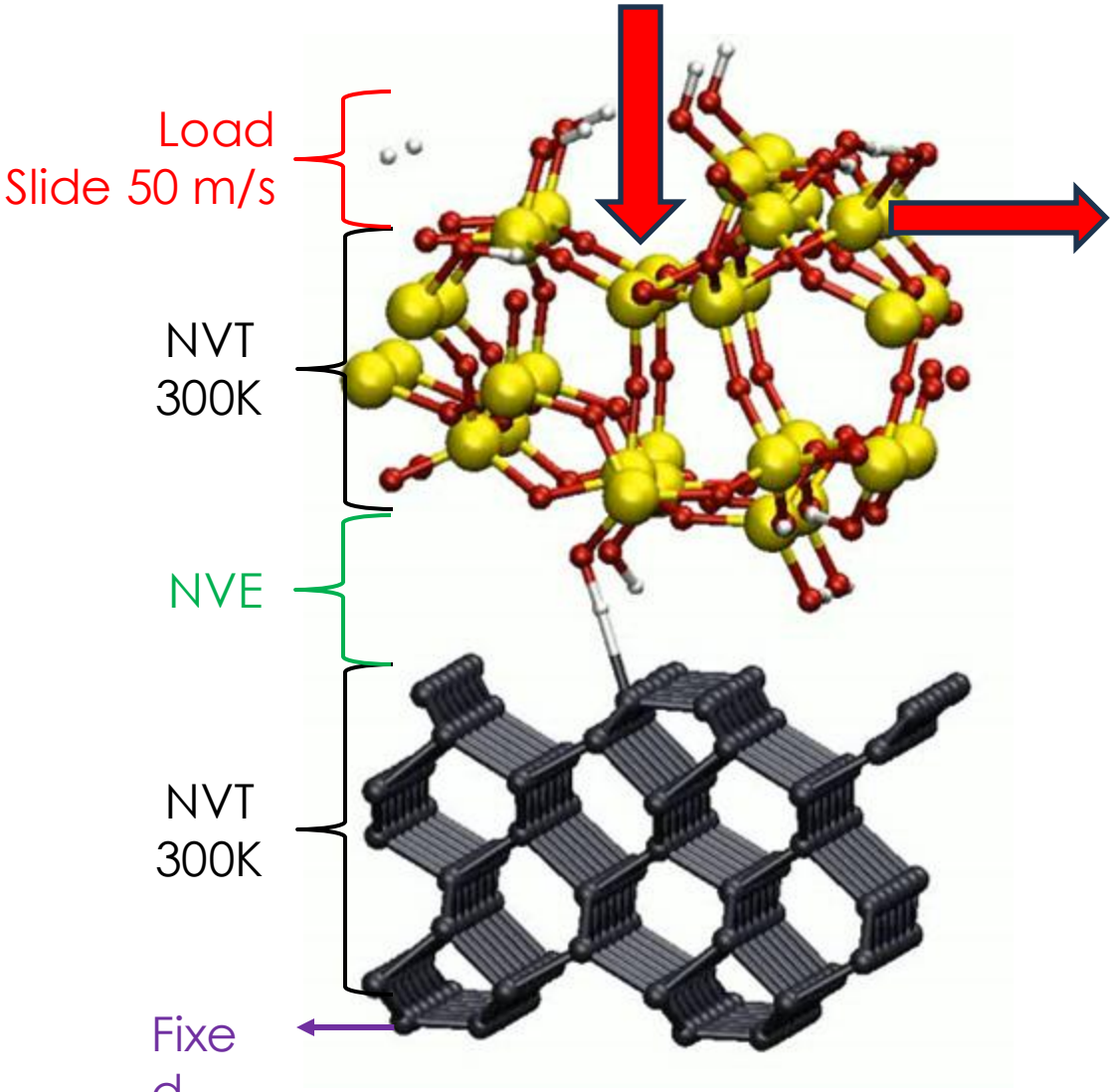

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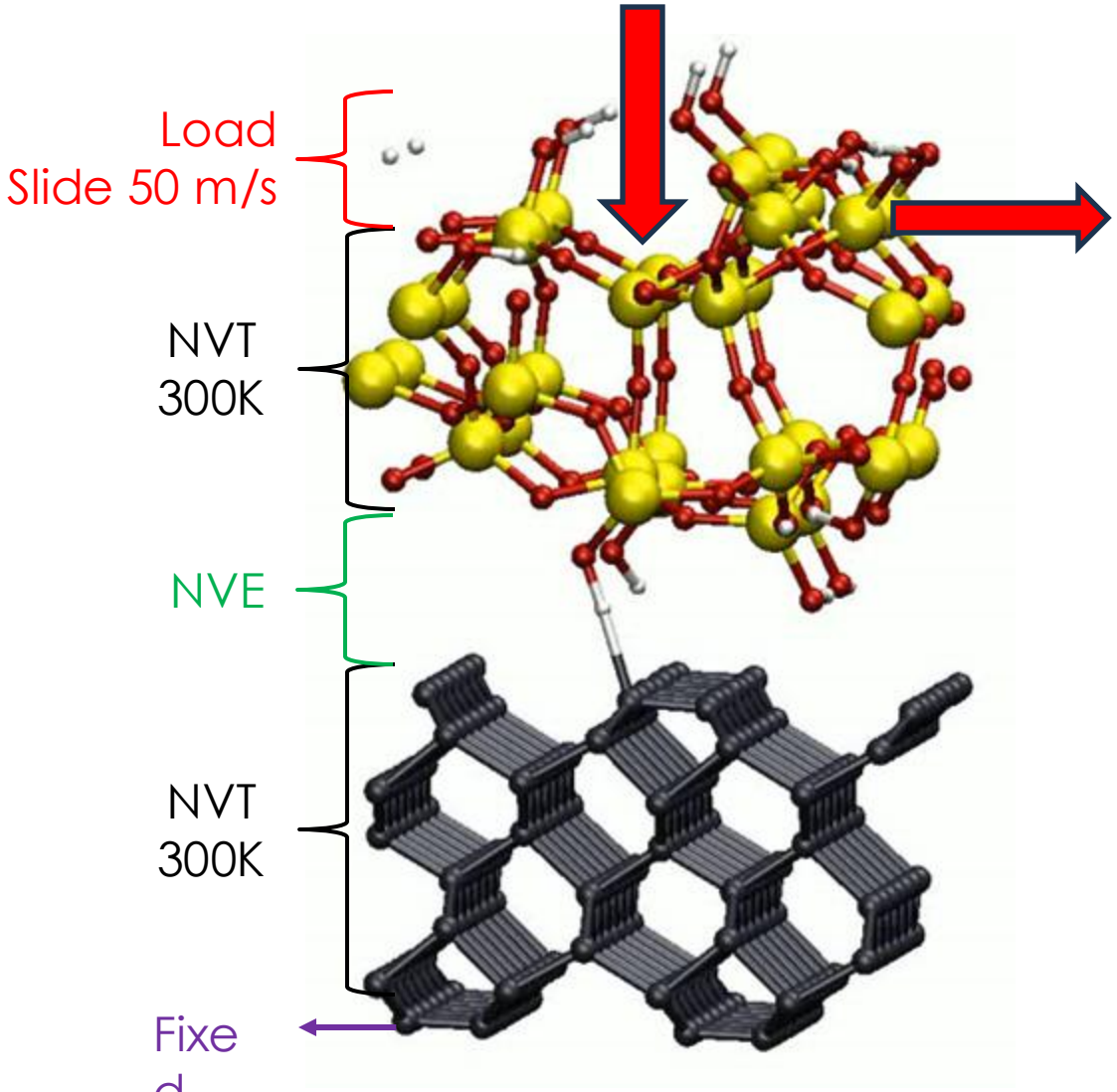

Silica-C(001) clean

Thermalization under load: 20ps
Sliding under load: 100ps

System of interest:

- Silica-C(001)
- Silica-C(110)
- Silica-reconstructed C(111)

Each diamond surface can have three different passivations: clean, 50% H and 50% H/OH

Download the Google Colab notebook

- Prerequisite: having a Google account

- Open the following link https://tinyurl.com/2ff66ftv in a web browser, download it locally and add in your Google Colab page (https://colab.research.google.com/). Then, follow the instruction within the notebook

- Open the following shared spreadsheet (https://tinyurl.com/5599a4dj) to add the data obtained at the end of the tutorial

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