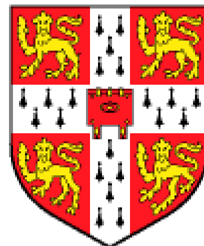
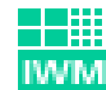
Development of a classical force field for the hydroxylated Si surface

D.J. Cole[1], M.C. Payne[1], L. Colombi Ciacchi[2,3]

[1] Theory of Condensed Matter Group, Cavendish Laboratory, Cambridge, U.K.
[2] Institute for Reliability of Systems and Devices, Karlsruhe, Germany
[3] Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany

TCM





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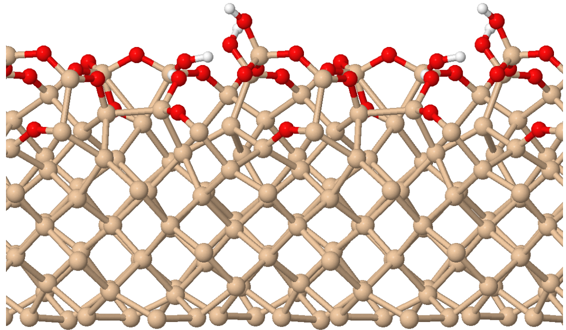
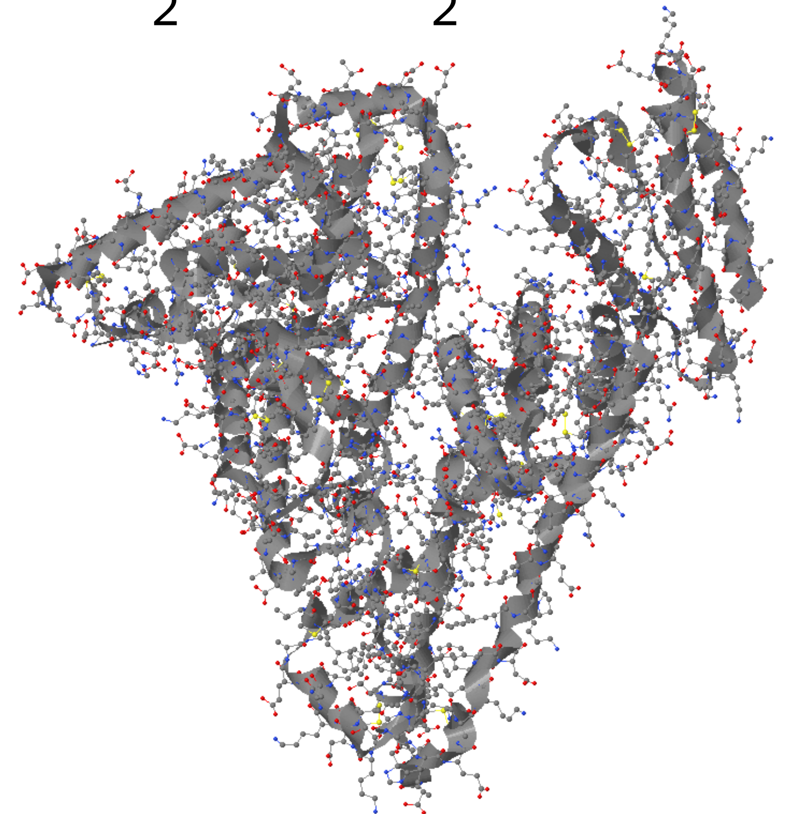
Introduction

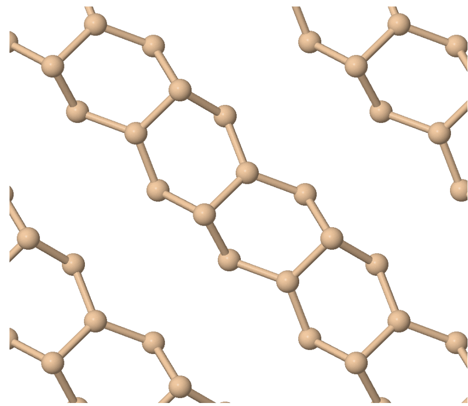


- Si-based MEMS devices form hydroxylated surface in presence of O_2 and H_2O
- Aim to study effects of surface chemistry on protein binding modes
- Need to develop classical force field for Si surface



Oxidation of the Si surface

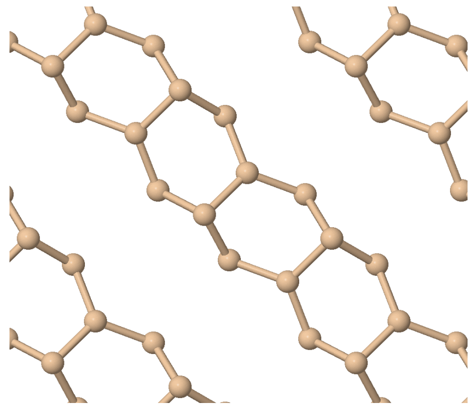
- Tensile stress development



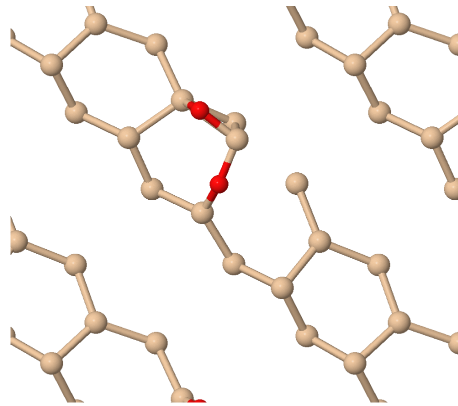
Θ=0.00 g=0.81N/m

Oxidation of the Si surface

- Tensile stress development



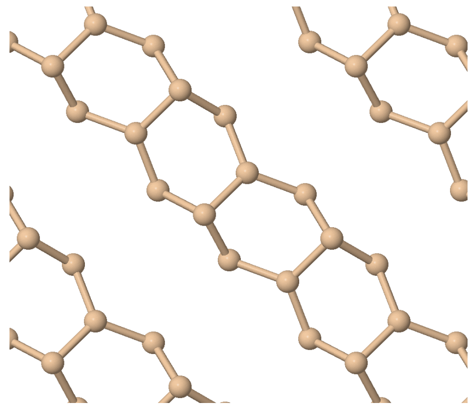
$\Theta=0.00$ g=0.81N/m



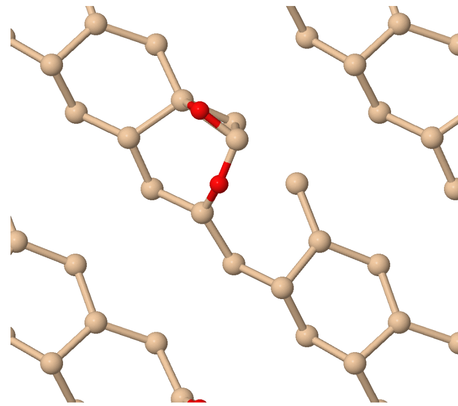
$\Theta=0.25$ g=0.47N/m

Oxidation of the Si surface

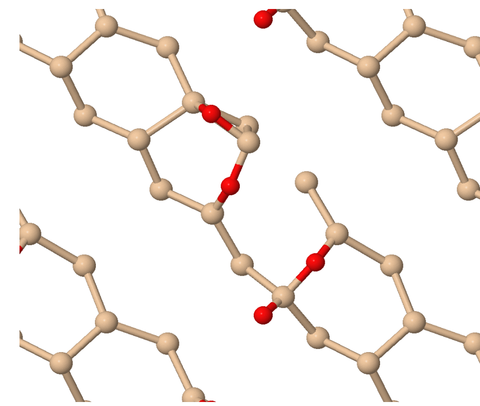
- Tensile stress development



$\Theta=0.00$ $g=0.81N/m$



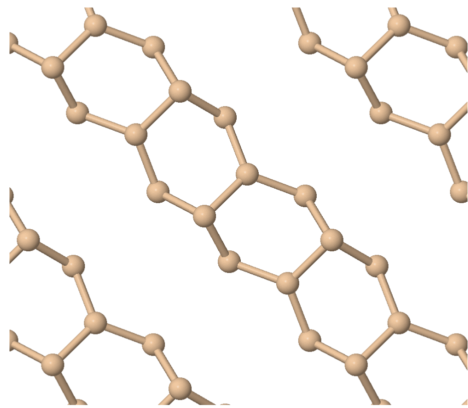
$\Theta=0.25$ $g=0.47N/m$



$\Theta=0.50$ $g=0.50N/m$

Oxidation of the Si surface

- Tensile stress development



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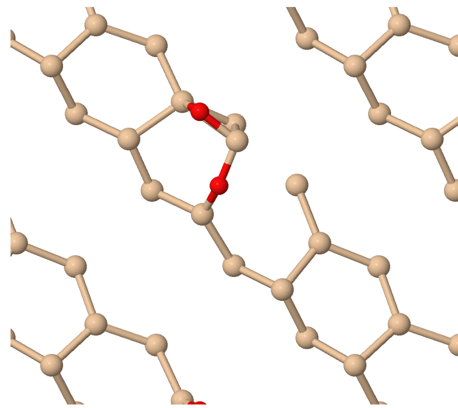

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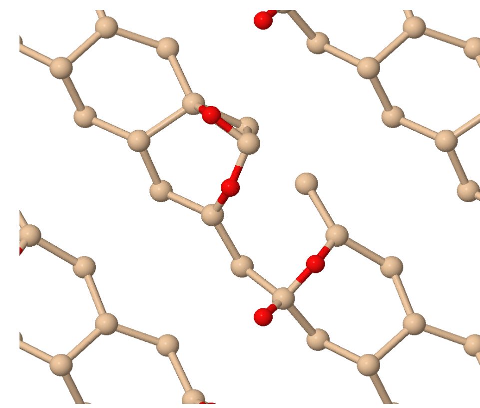

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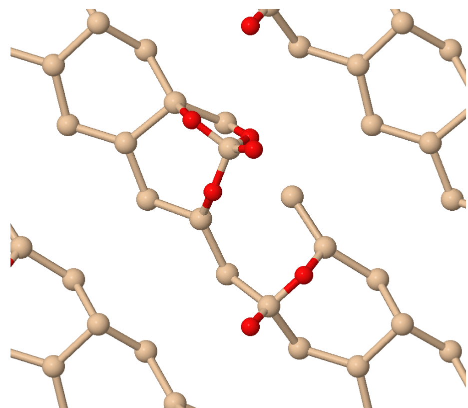
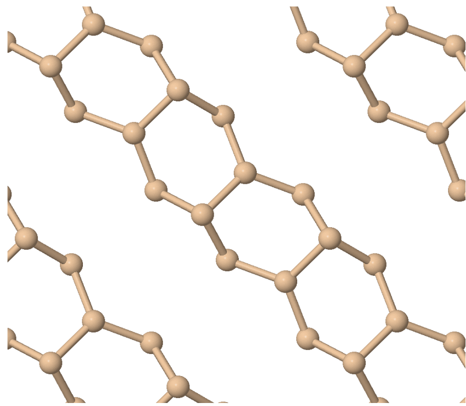


Θ=0.75 g=0.05N/m

Oxidation of the Si surface

- Tensile stress development



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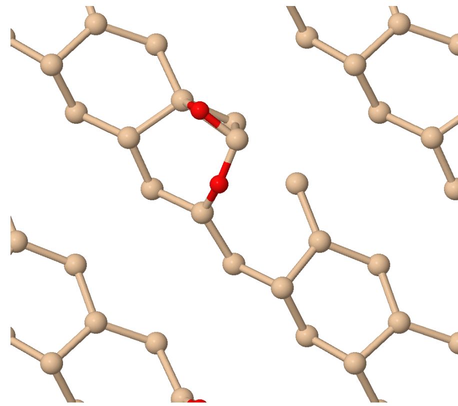

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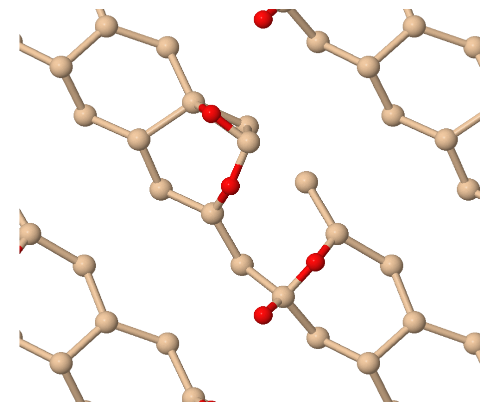

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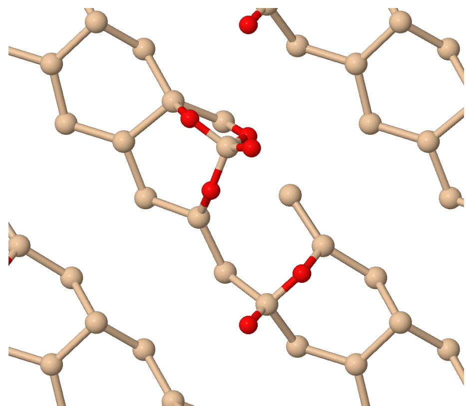

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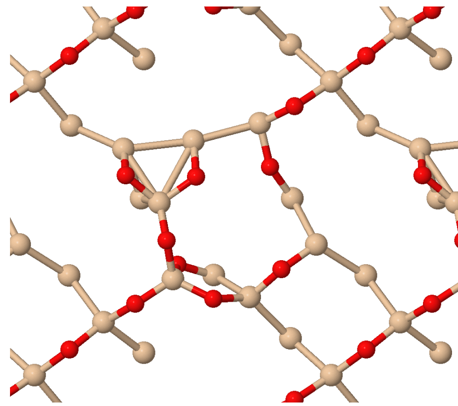
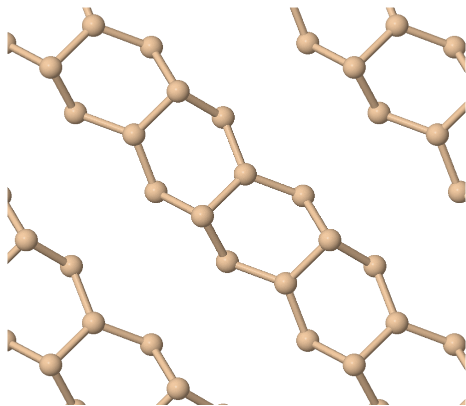


Θ=1.25 g=1.28N/m

Oxidation of the Si surface

- Tensile stress development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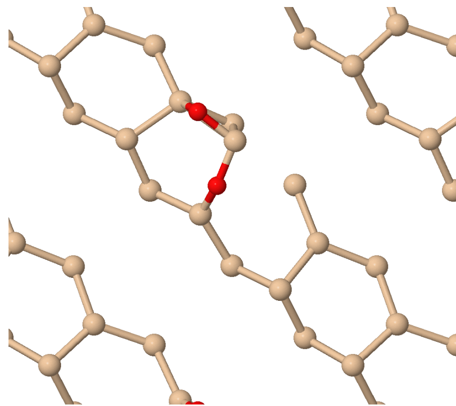
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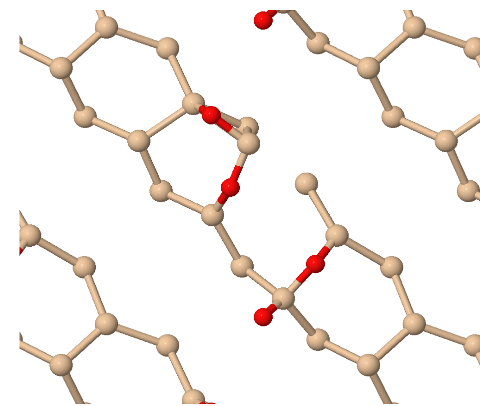
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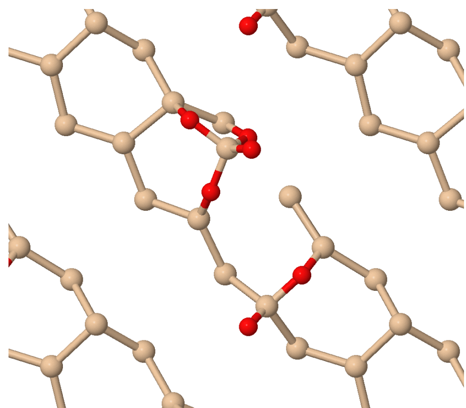
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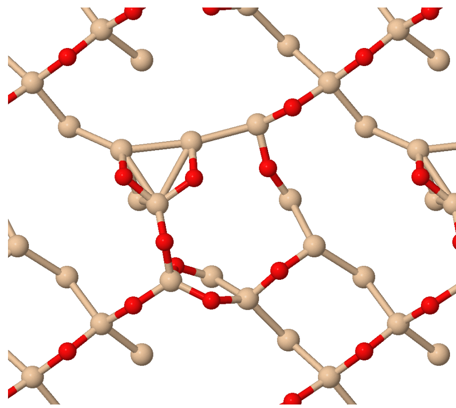
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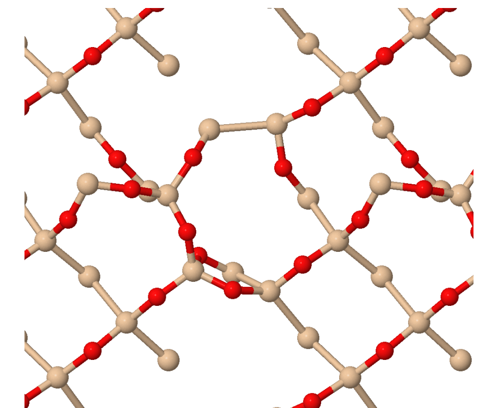
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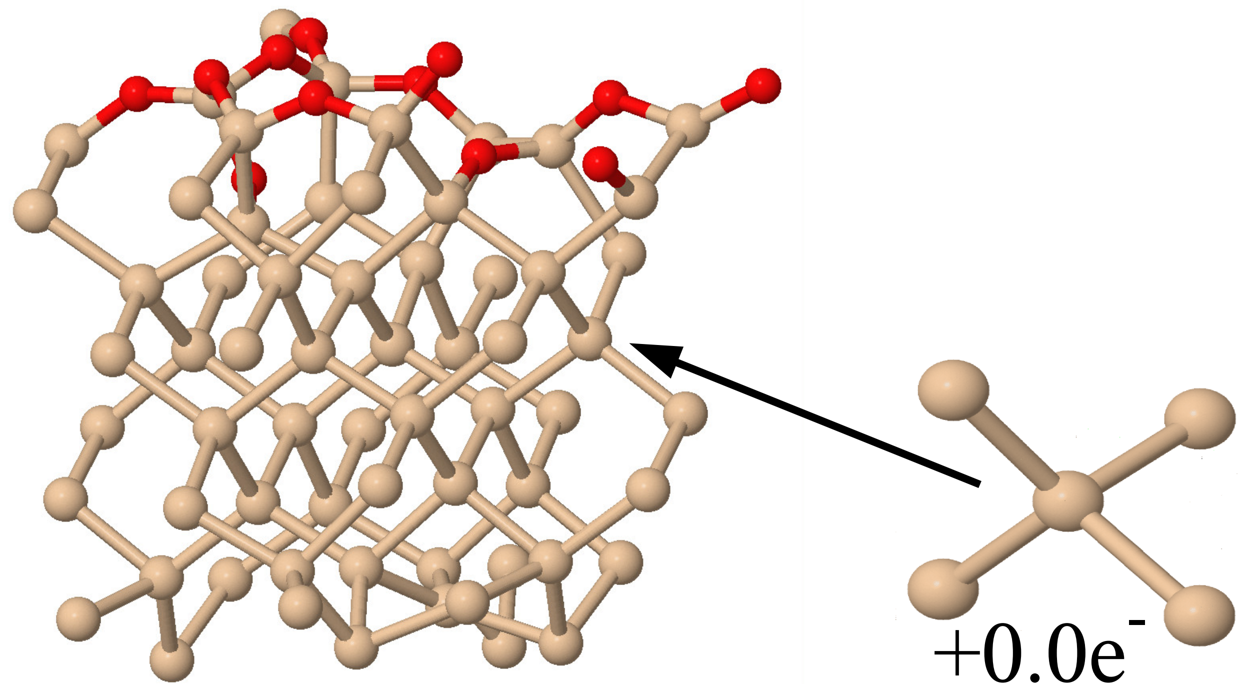
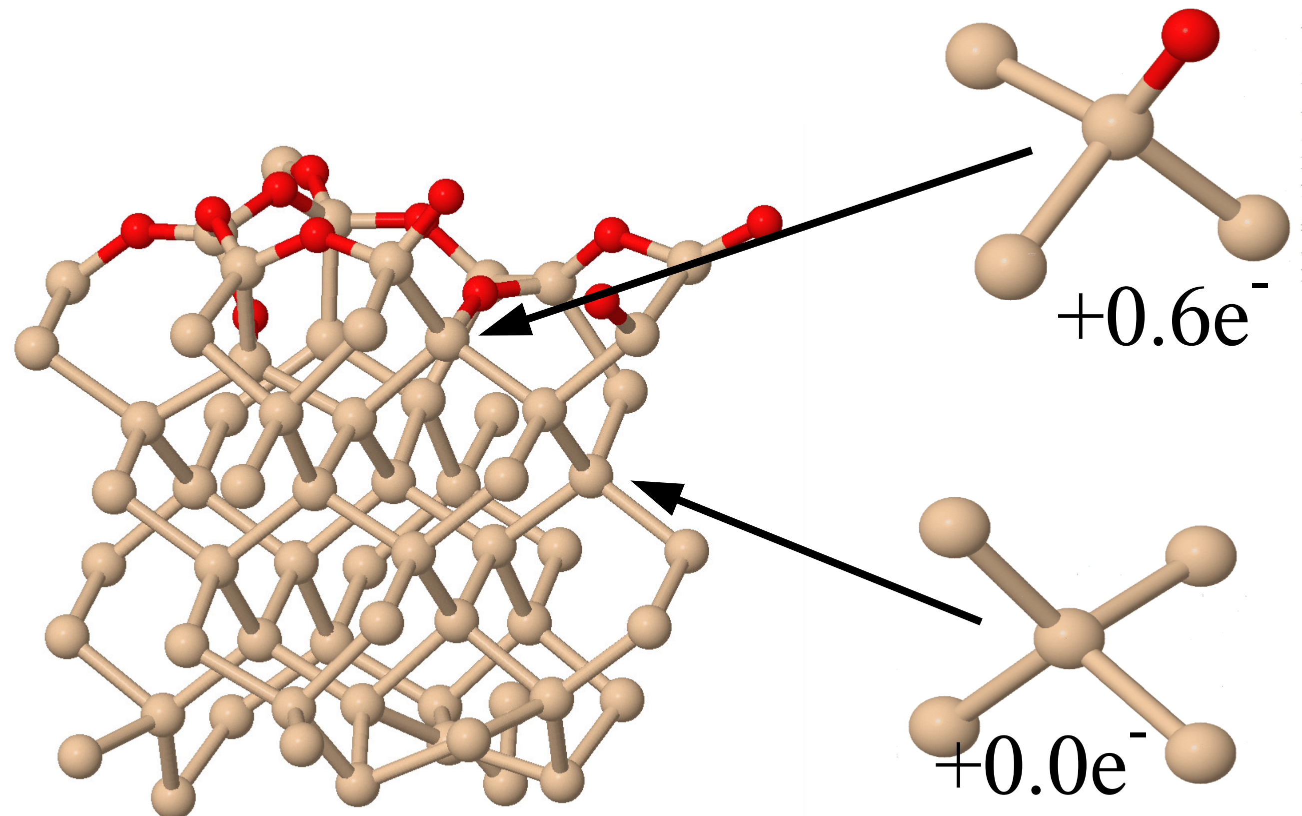
Oxidation of the Si surface

- Mulliken charges



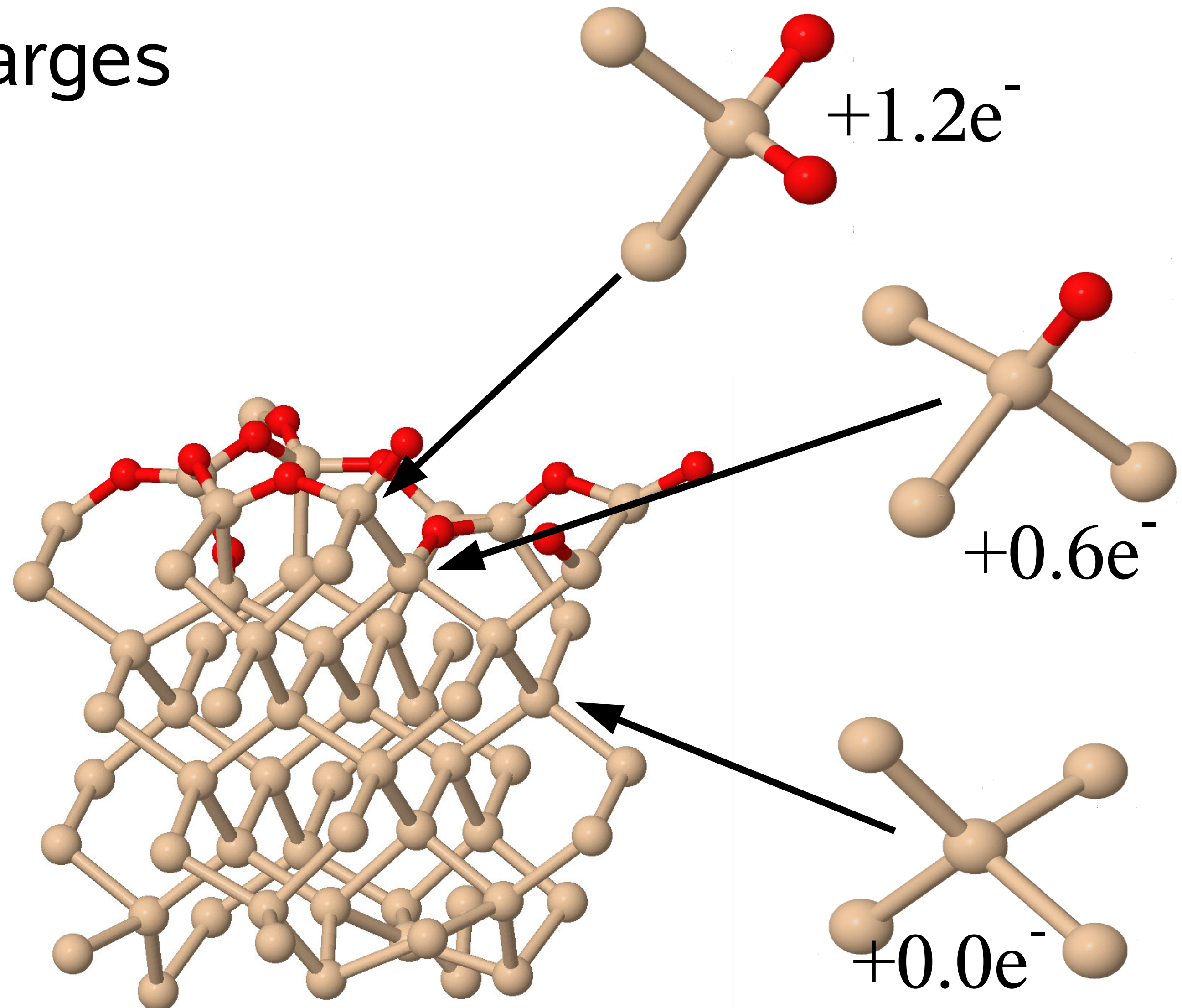
Oxidation of the Si surface

- Mulliken charges



Oxidation of the Si surface

- Mulliken charges



Oxidation of the Si surface

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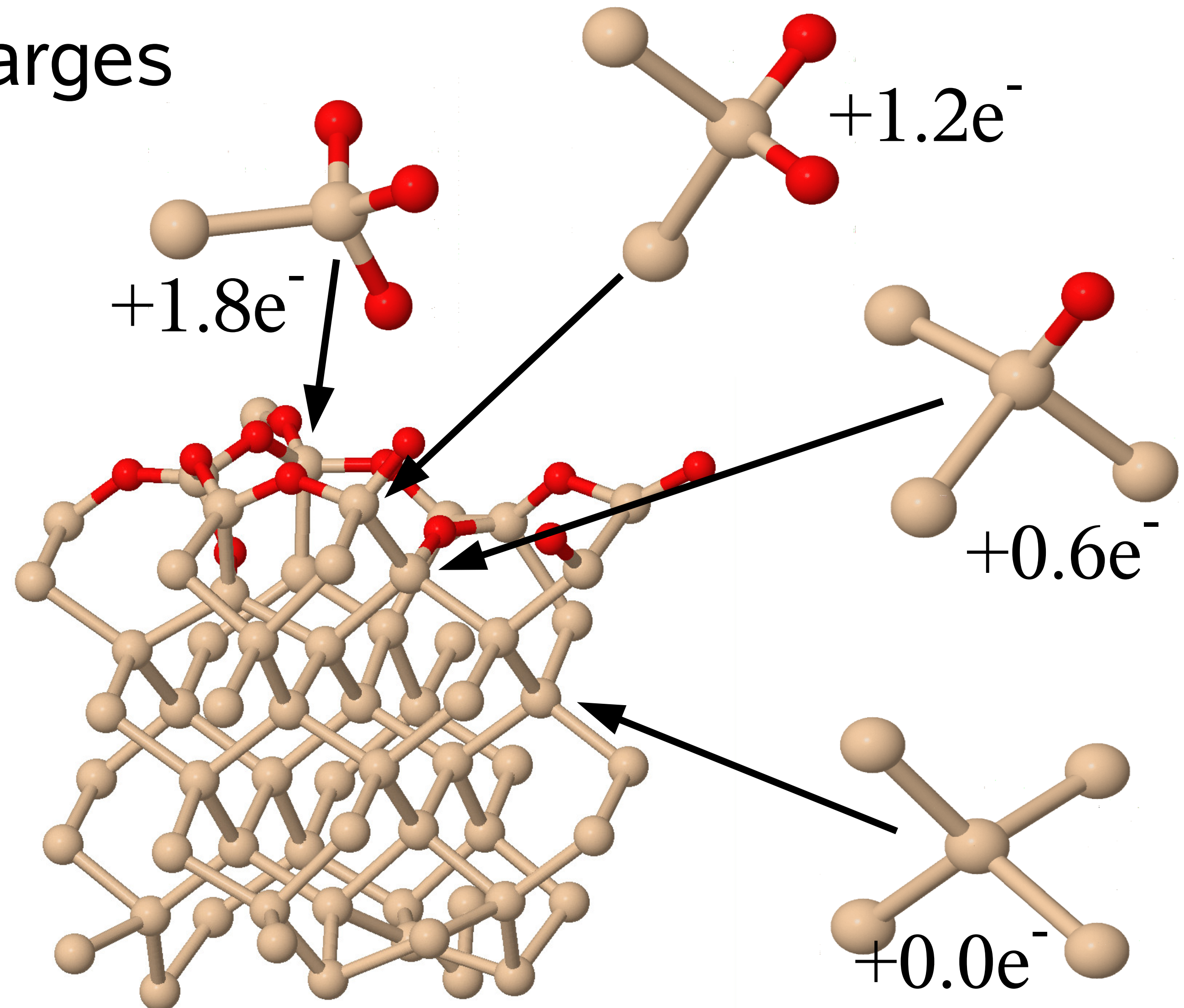

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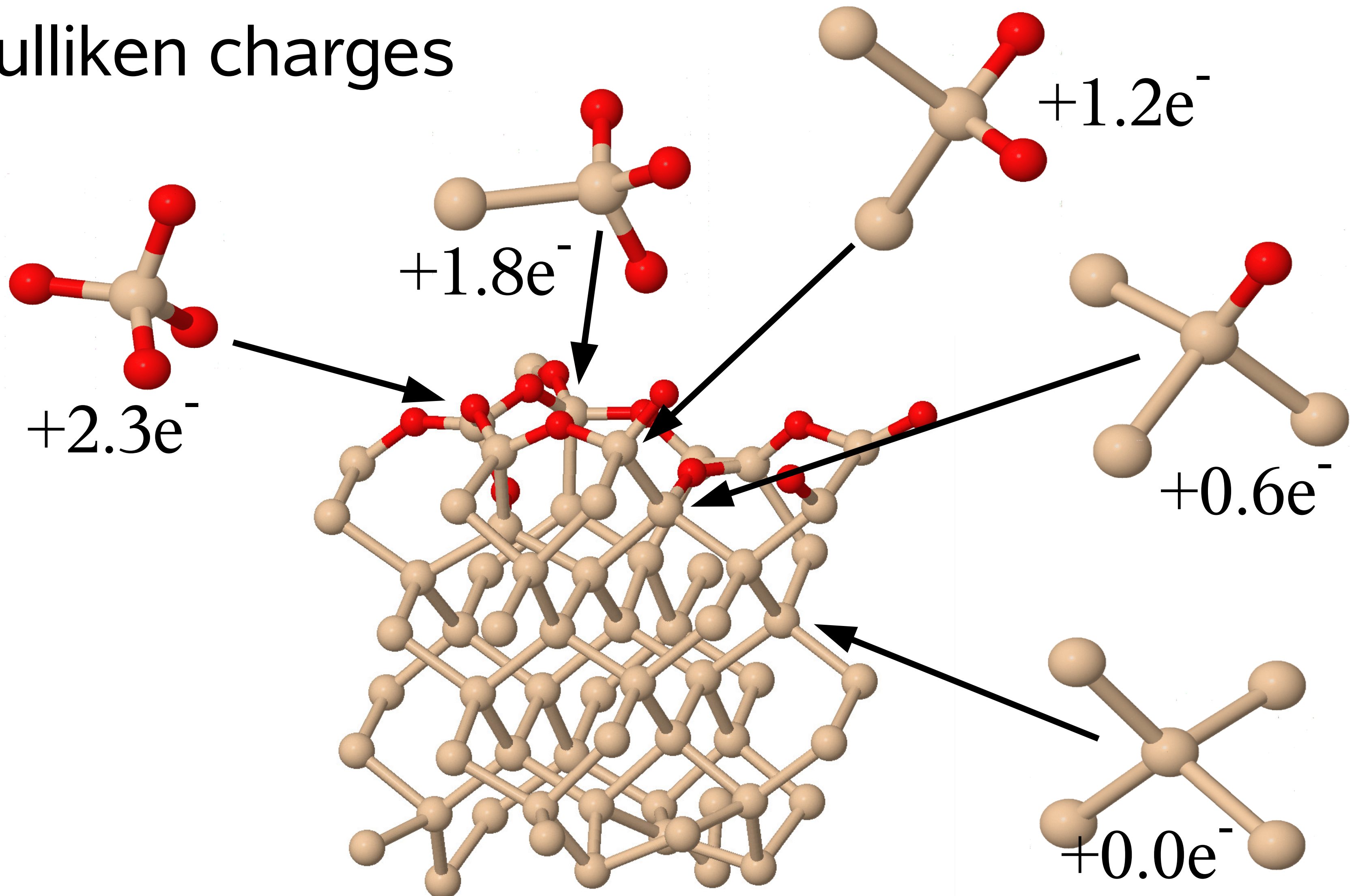
- Mulliken charges



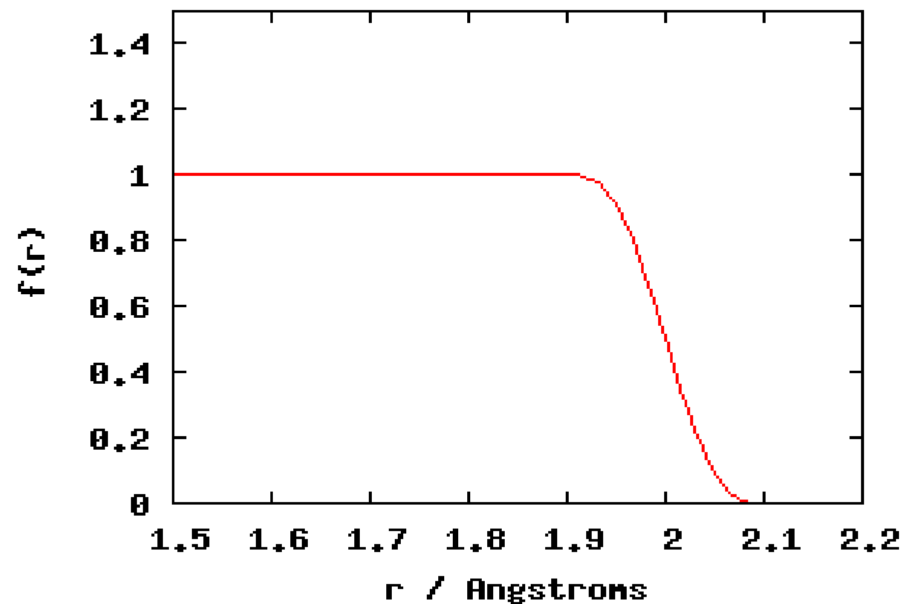
Summary so far

- High tensile surface stress in the native oxide
- Si charges increase linearly with number of O nearest neighbours
- Develop a charge-based classical force field, fit to ab-initio structure and tensile stress

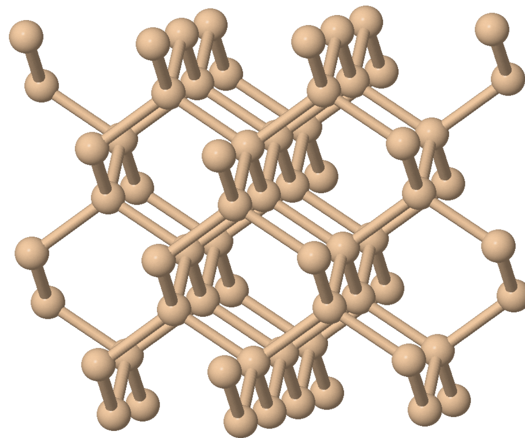
A classical force field

$$q_{Si} = +0.4 \sum_{O} f(r)$$

$$q_{O} = -0.4 \sum_{Si} f(r)$$



A classical force field

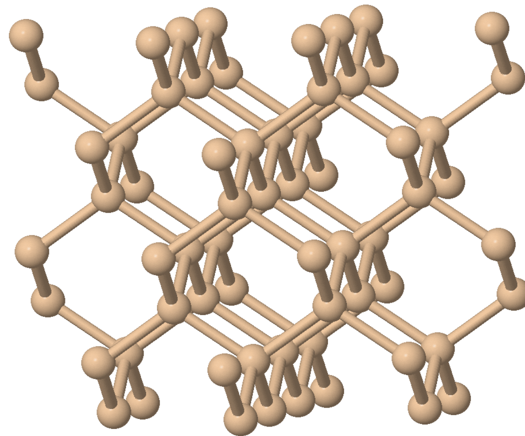


$$V_{Si-Si'} = A[Br^{-4} - 1]\exp(\sigma(r-a)^{-1})$$

$$V_{ijk} = \lambda\exp[\gamma_1(r_{ij}-d_1)^{-1}+\gamma_2(r_{ik}-d_2)^{-1}](cos\theta_{jik}-cos\theta_0)^2$$

F.H. Stillinger and T.A. Weber, Phys. Rev. B **31**, 5262 (1985)

A classical force field



$$V_{Si-Si'} = A(q_{Si}, q_{Si'})[Br^{-4} - 1]\exp(\sigma(r-a)^{-1}) f(r) + \frac{q_{Si} q_{Si'}}{r}$$

$$V_{ijk} = \lambda \exp[\gamma_1 (r_{ij} - d_1)^{-1} + \gamma_2 (r_{ik} - d_2)^{-1}](cos\theta_{jik} - cos\theta_0)^2 f(r)$$

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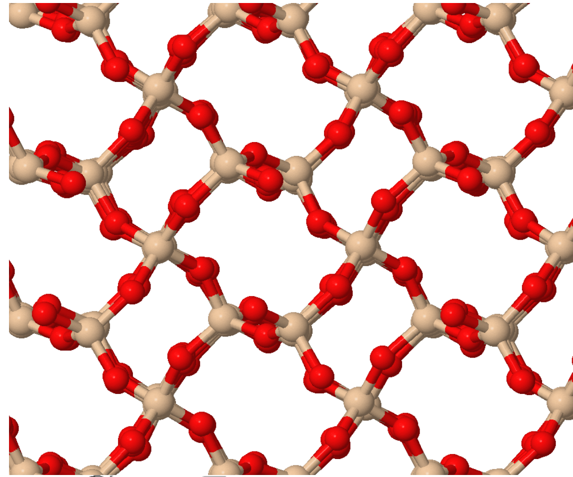
A classical force field



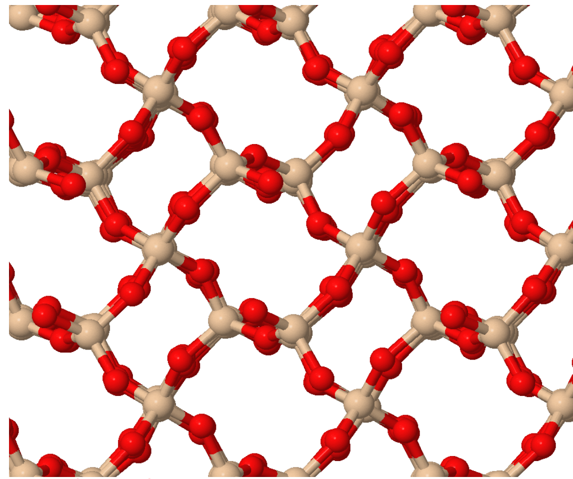
$$V_{Si-O} = \frac{C}{r^9} - \frac{D}{r^4}\exp(-r/b) + \frac{q_{Si}q_O}{r}$$

$$V_{O-O'} = \frac{H}{r^7} - \frac{J}{r^4}\exp(-r/b) + \frac{q_O q_{O'}}{r}$$

$$V_{ijk} = \lambda \exp[\gamma_1(r_{ij} - d_1)^{-1} + \gamma_2(r_{ik} - d_2)^{-1}](cos\theta_{jik} - cos\theta_0)^2$$

P. Vashishta, R.K. Kalia and J.P. Rino, Phys. Rev. B **41**, 12197 (1989)

A classical force field



$$V_{Si-O} = \frac{C(q_{Si})}{r^9} - \frac{D}{r^4}\exp(-r/b) + \frac{q_{Si}q_O}{r}$$

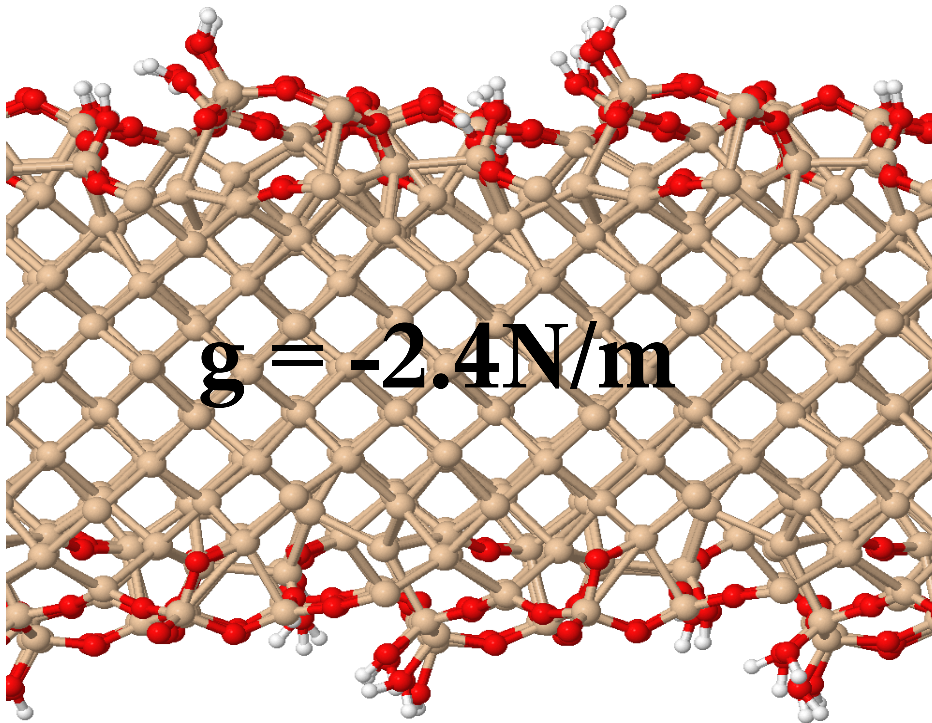
$$V_{O-O'} = \frac{H}{r^7} - \frac{J}{r^4}\exp(-r/b) + \frac{q_O q_{O'}}{r}$$

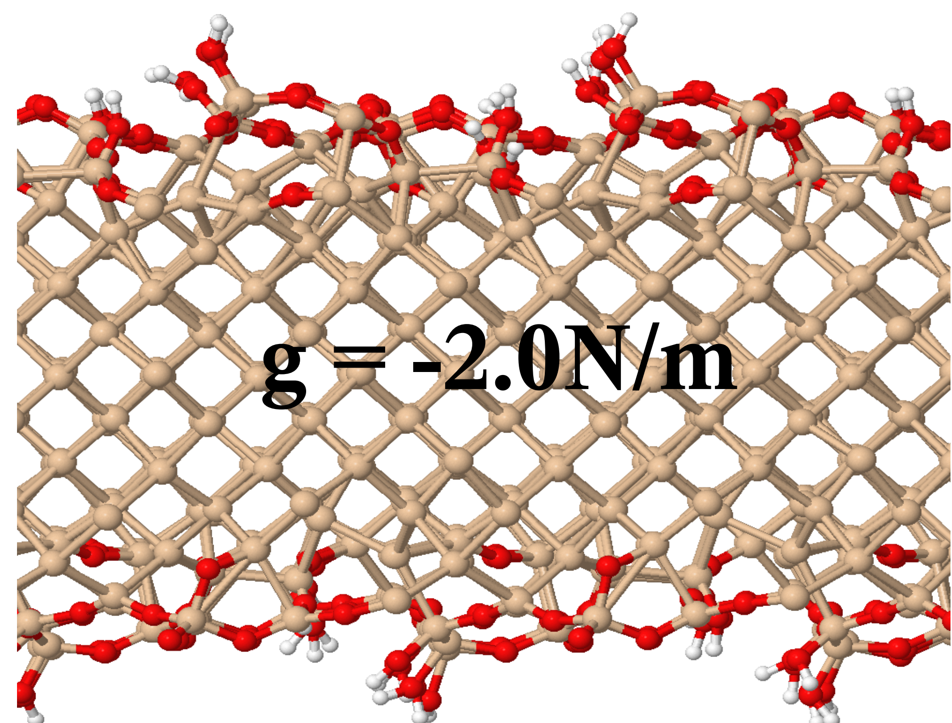
$$V_{ijk} = \lambda \exp[\gamma_1(r_{ij}-d_1)^{-1}+\gamma_2(r_{ik}-d_2)^{-1}](cos\theta_{jik}-cos\theta_0)^2$$

P. Vashishta, R.K. Kalia and J.P. Rino, Phys. Rev. B **41**, 12197 (1989)

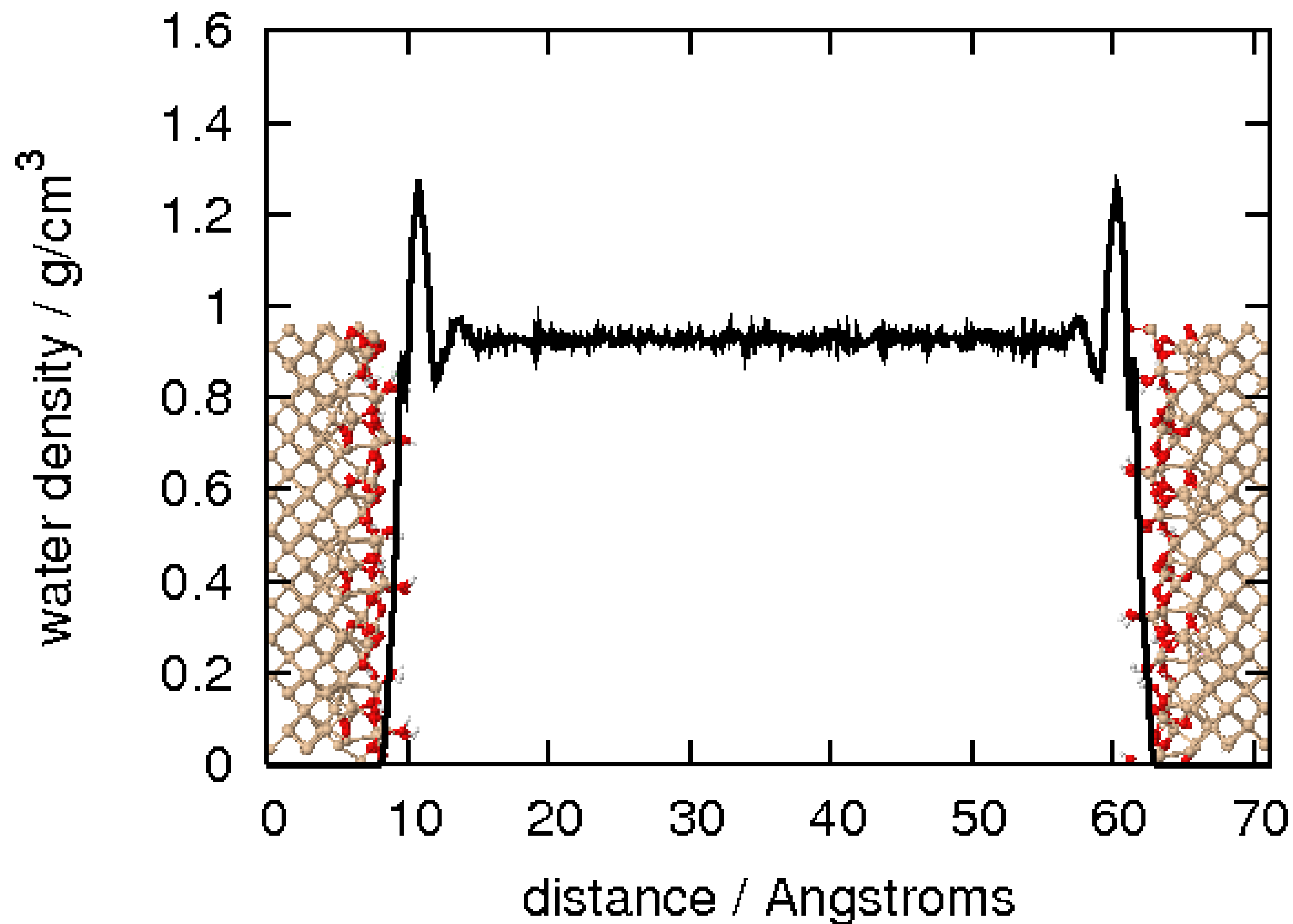
Hydroxylated surface results

	Ab-initio structure					Classical structure after 50ps MD at 300K				
	Bond length/Å		Bond angle			Bond length/Å		Bond angle		
	Si-O	Si-Si	O-Si-O	Si-Si-O	Si-Si-Si	Si-O	Si-Si	O-Si-O	Si-Si-O	Si-Si-Si
Si^{4+}	1.64	–	109°	–	–	1.63	–	109°	–	–
Si^{3+}	1.65	2.36	109°	109°	–	1.62	2.42	119°	96°	–
Si^{2+}	1.67	2.39	109°	108°	109°	1.63	2.45	139°	101°	109°
Si^{+}	1.70	2.38	–	108°	111°	1.65	2.39	–	108°	111°





Water layering



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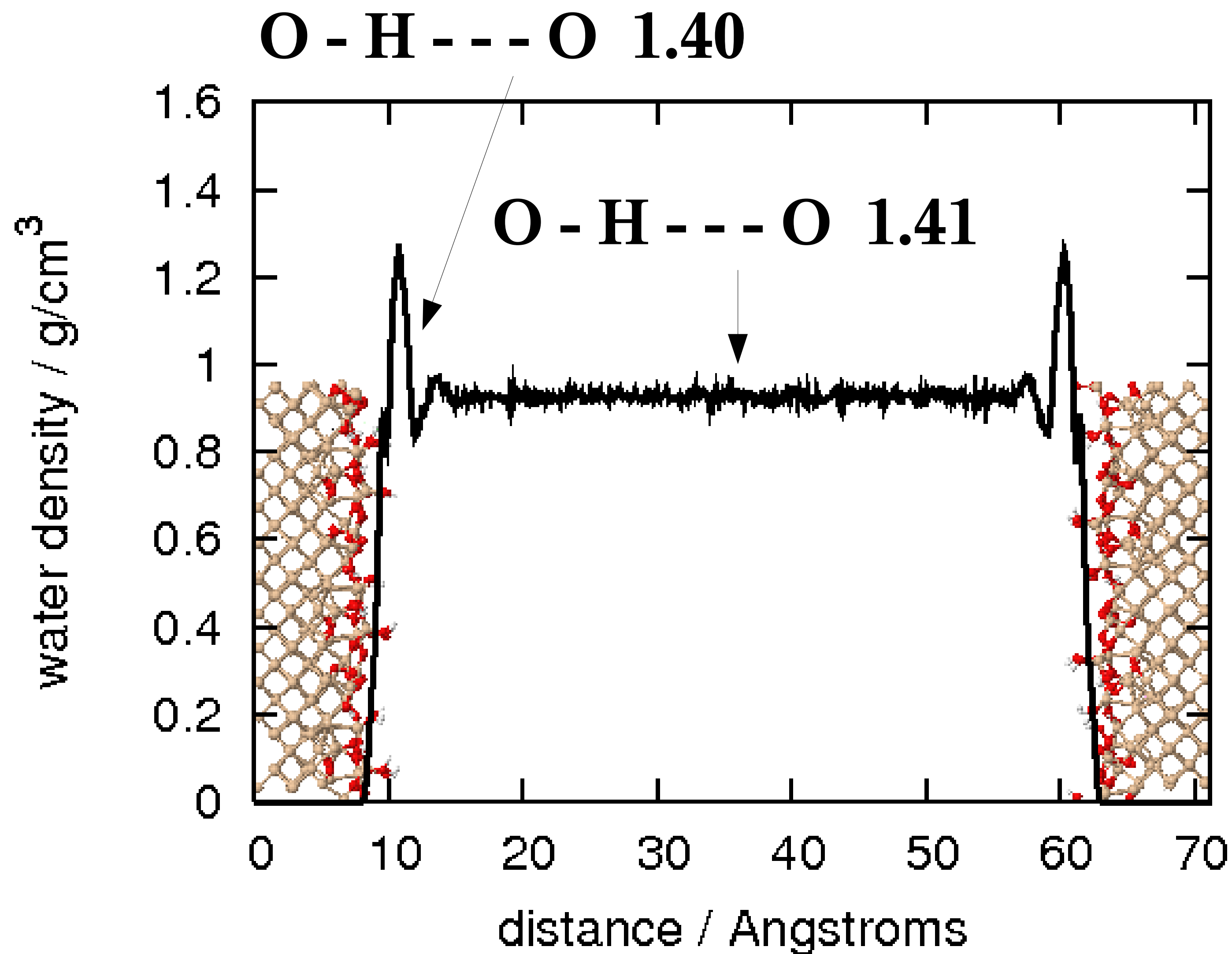
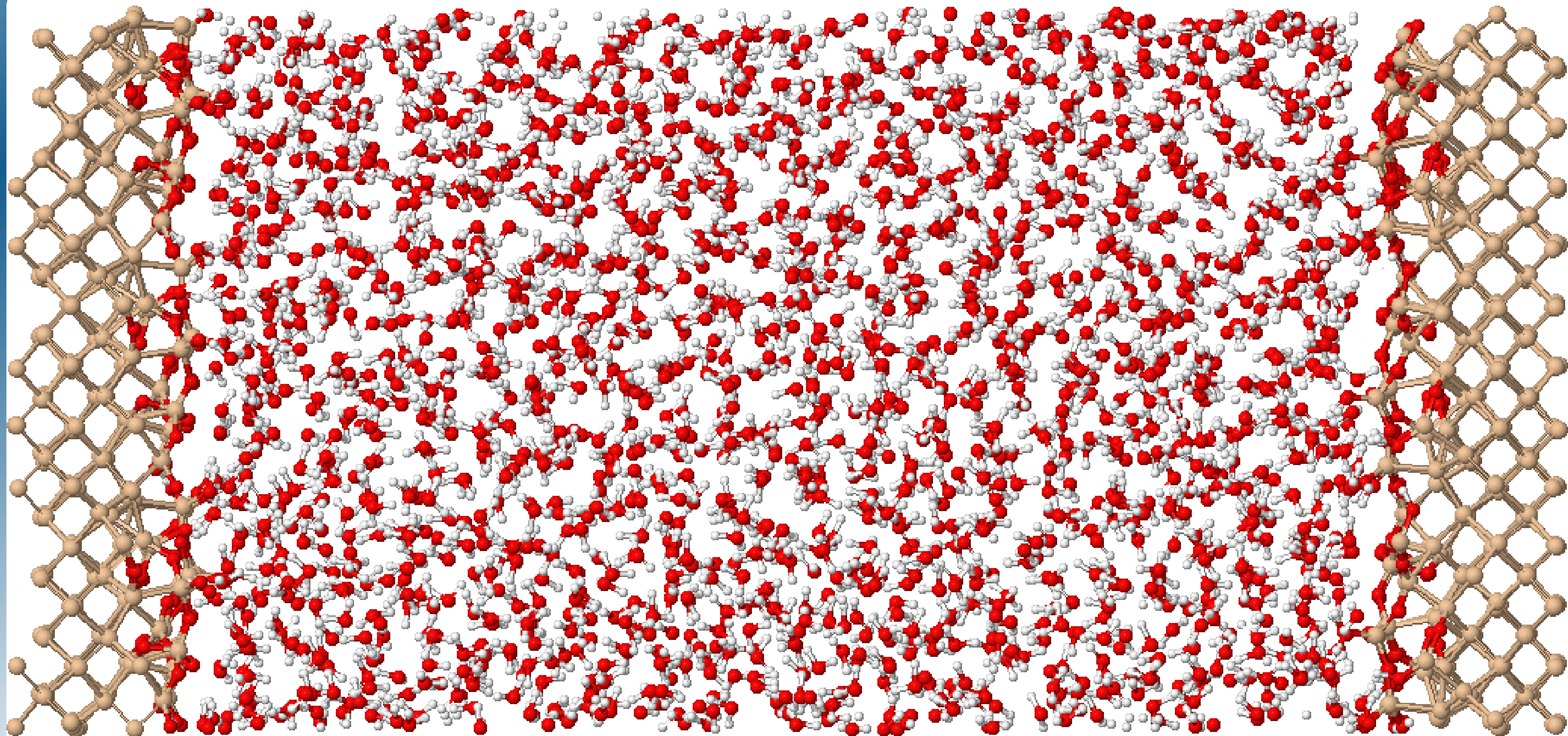


MEMS Wafer bonding

- Si wafer surface preparation – flat, clean, chemisorbed -OH, H-bonded H_2O
- Room temperature contact – assumed to be H-bonded network between surfaces
- High T annealing – desorbs H_2O and encourages siloxane bond formation

Wafer bonding



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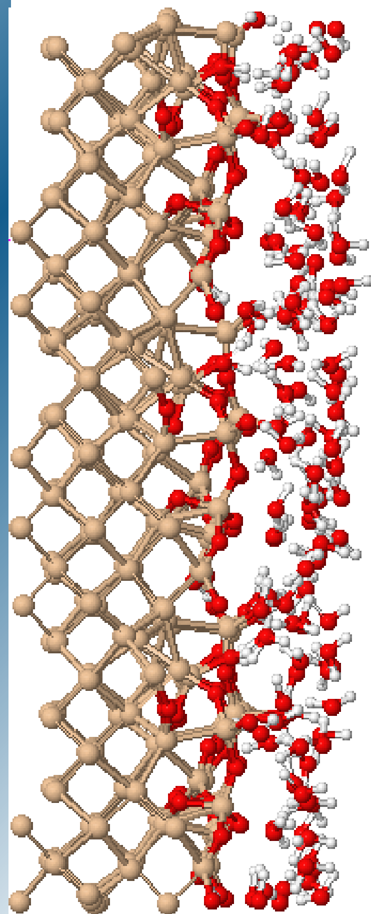

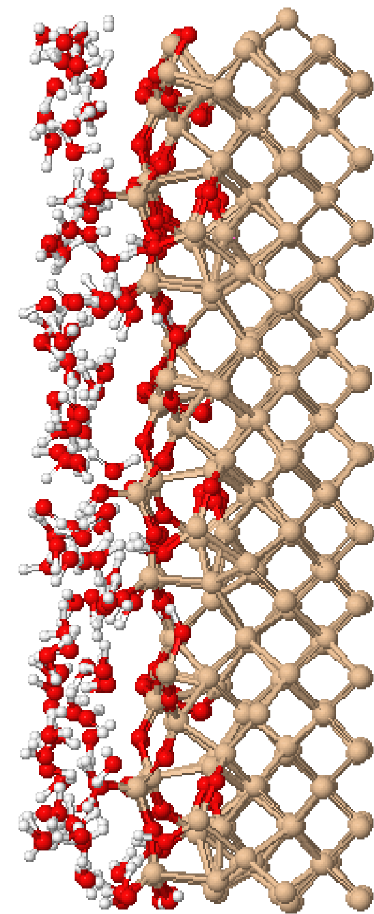

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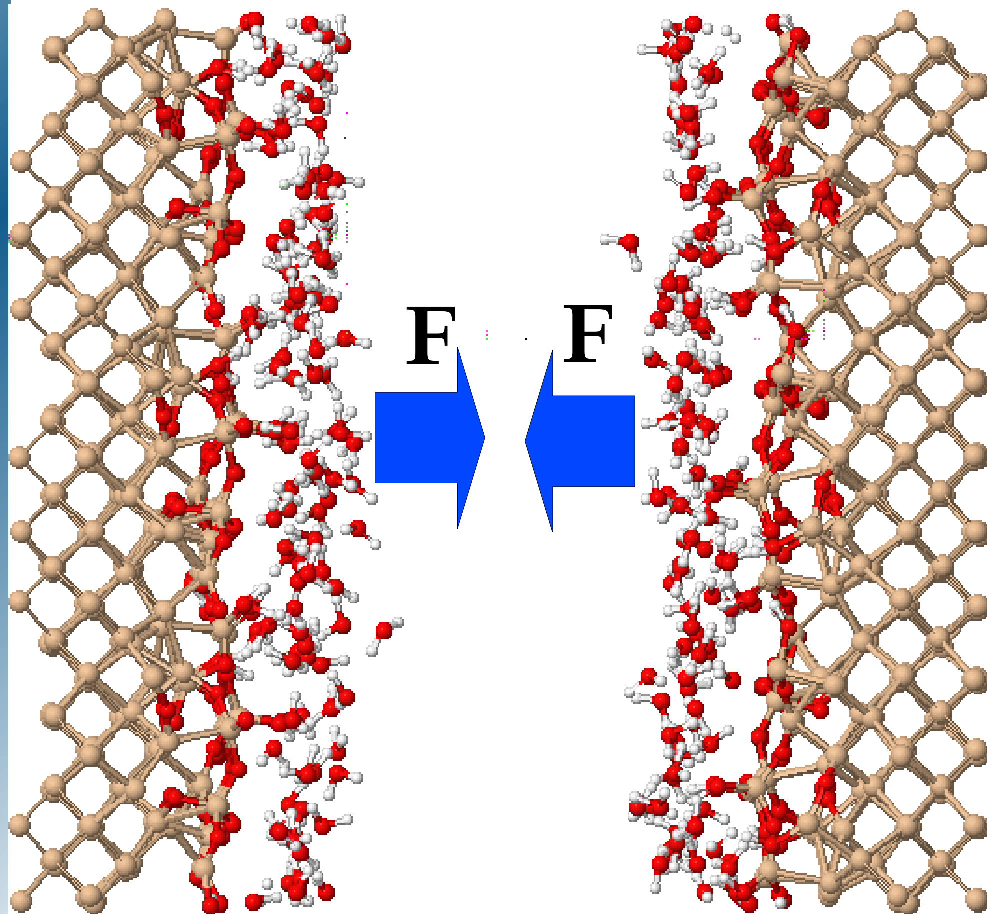

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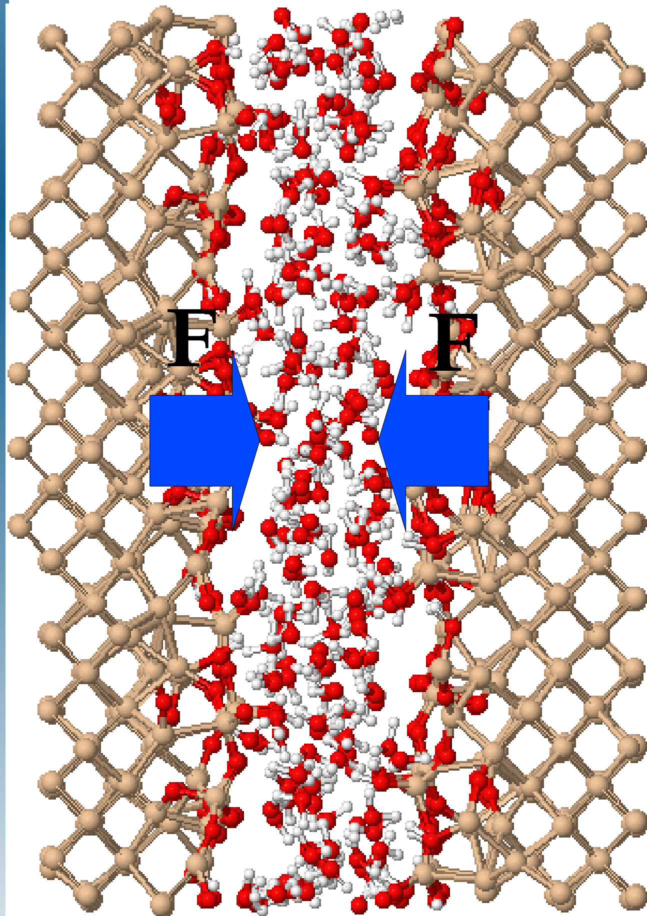

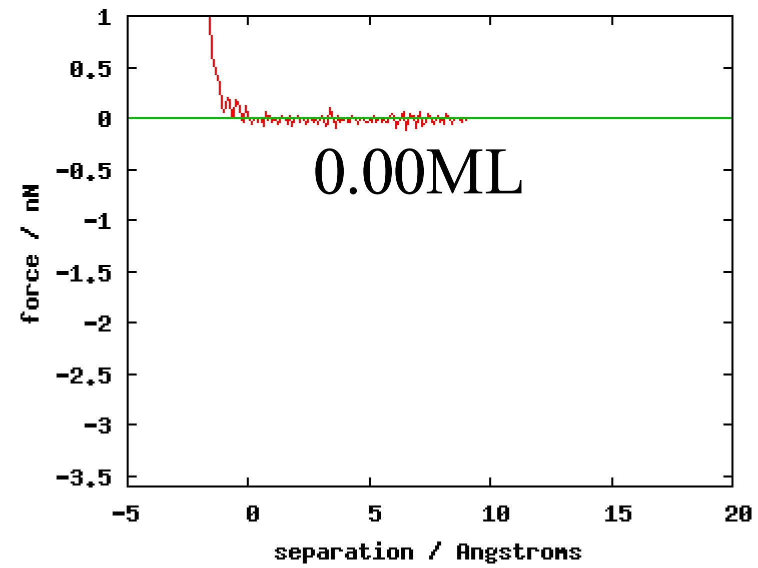

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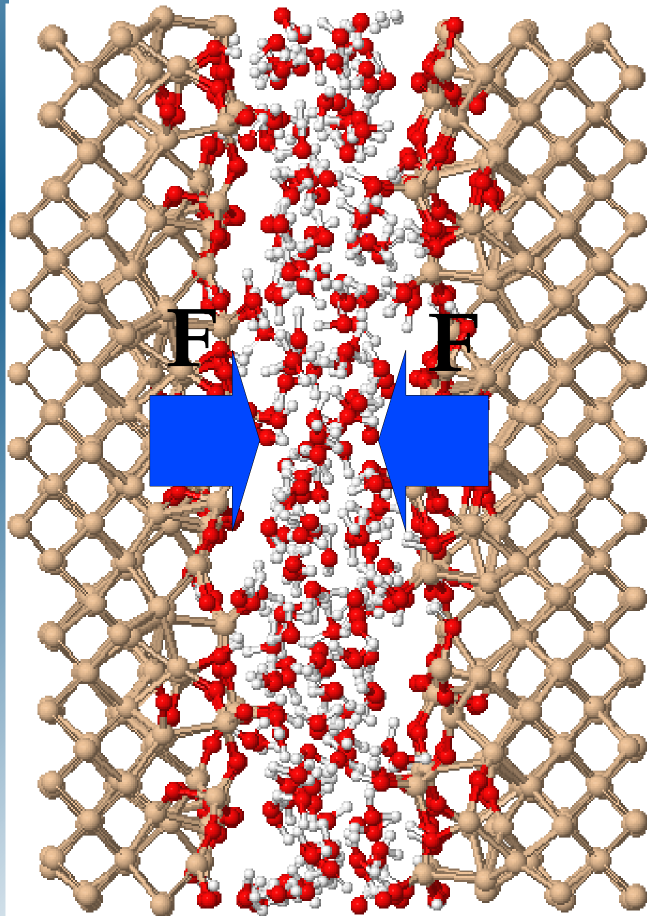

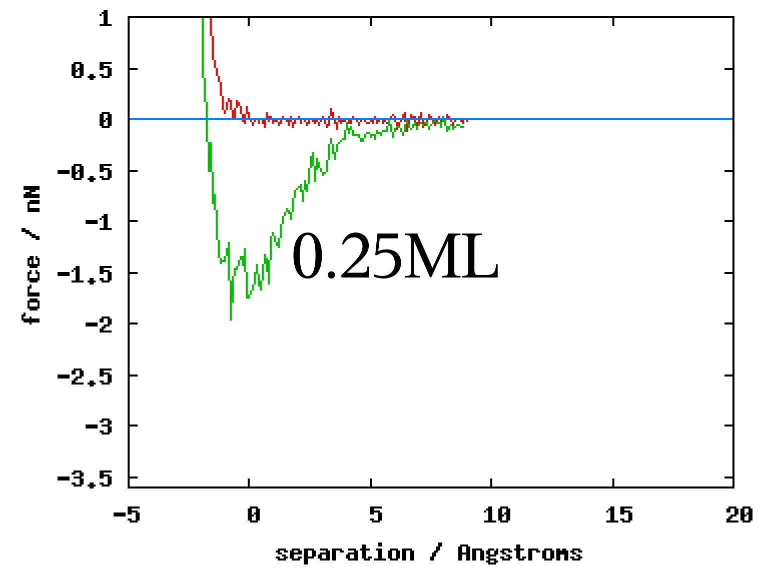

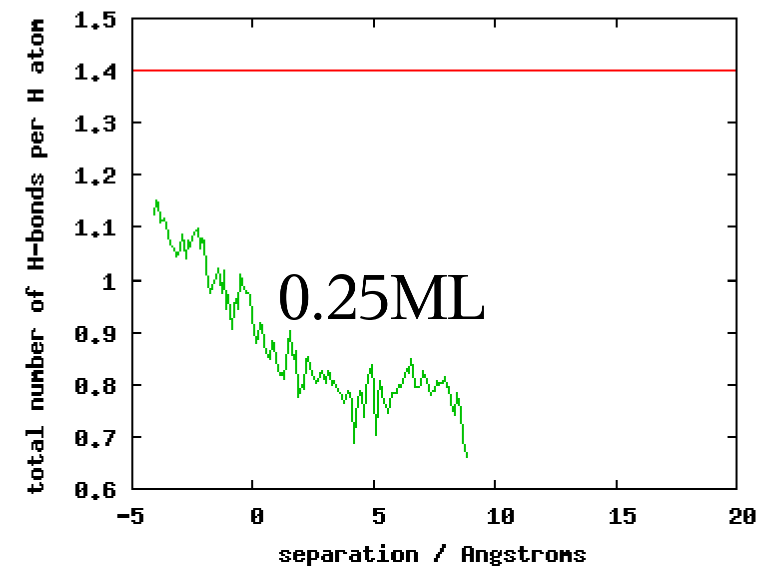

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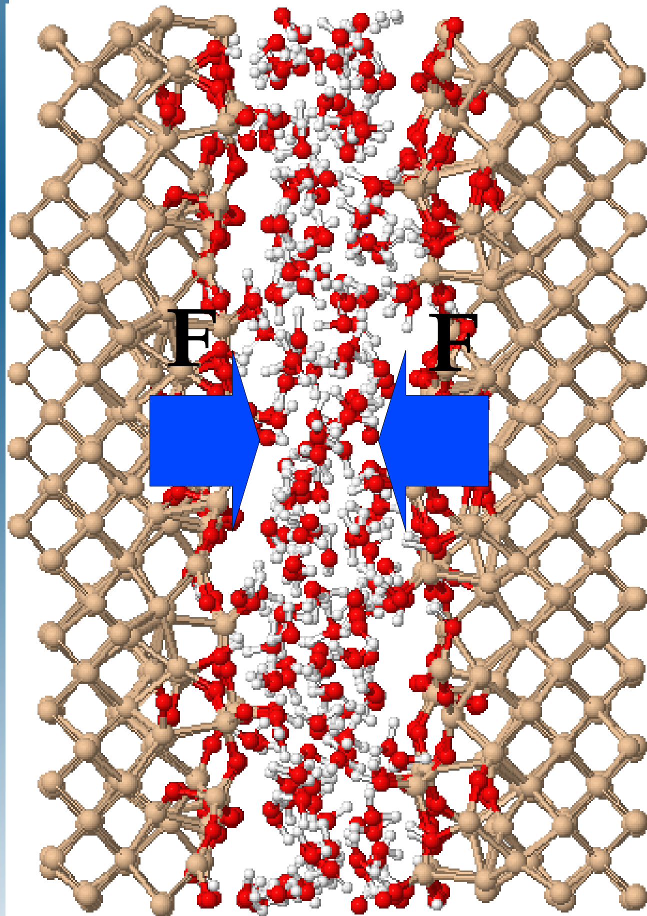

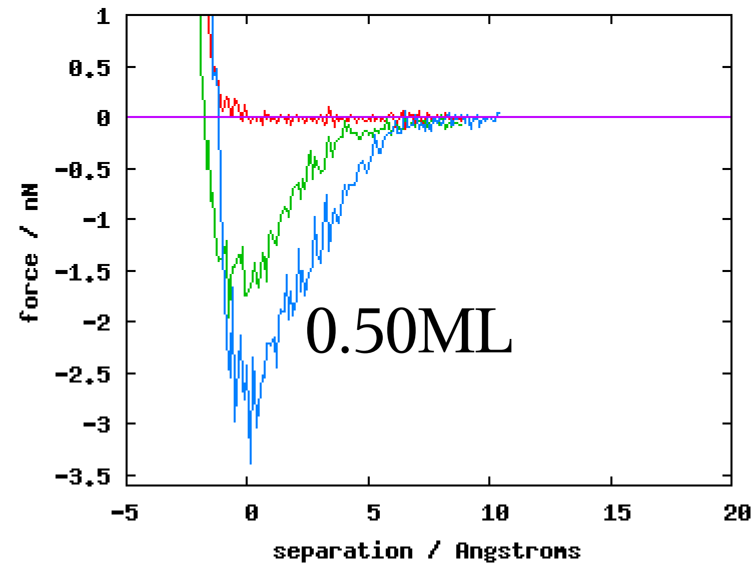

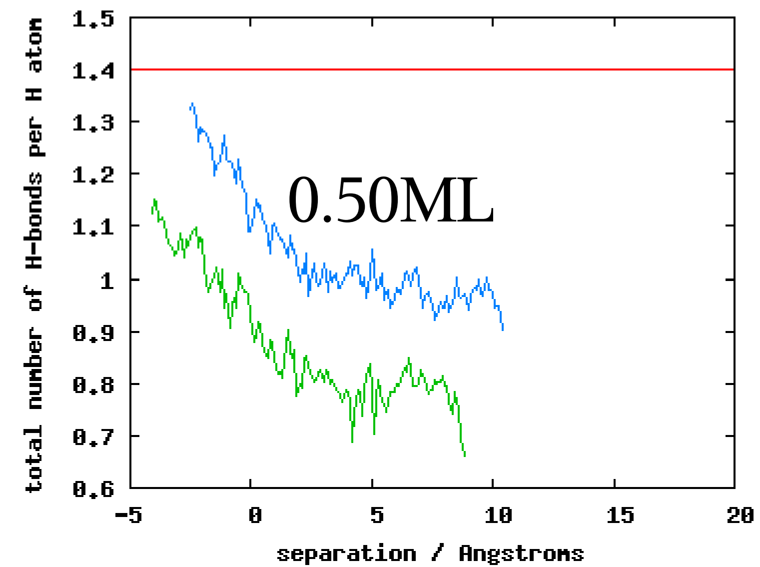

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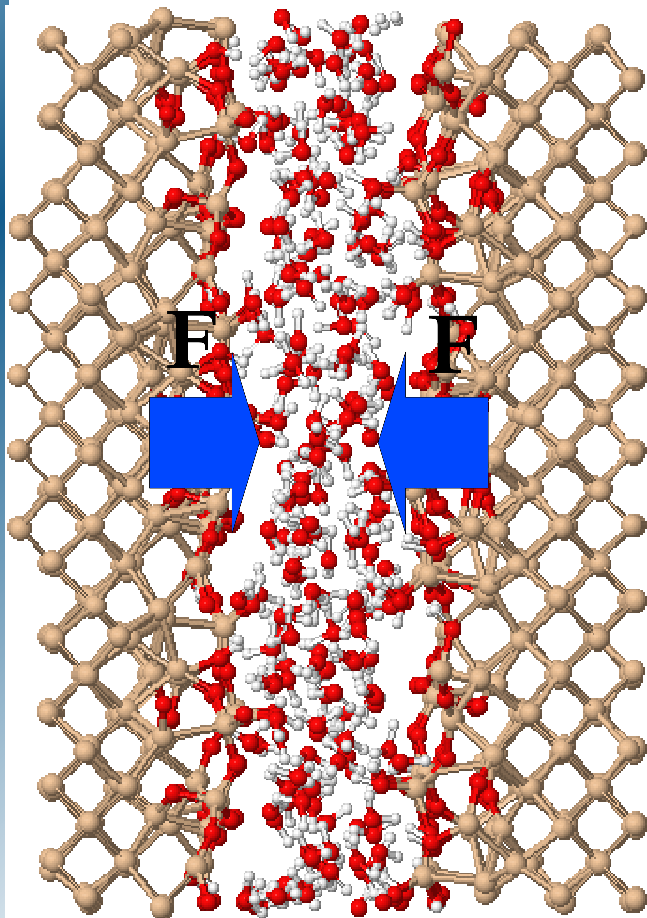

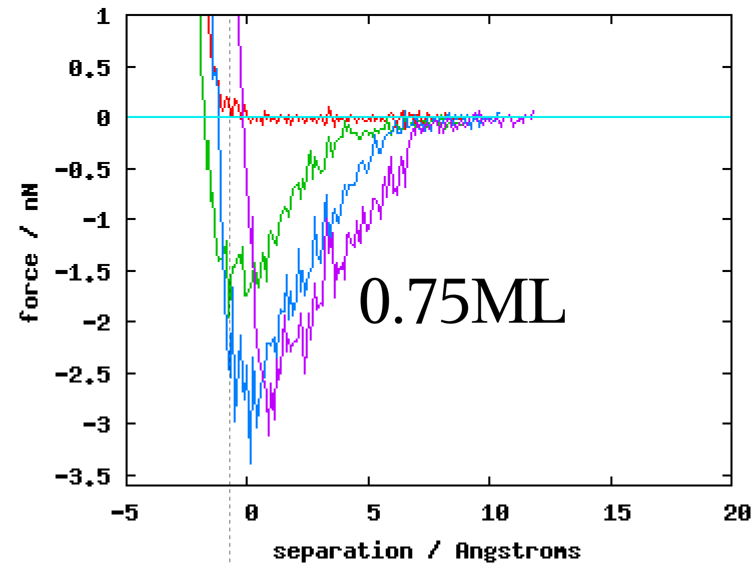

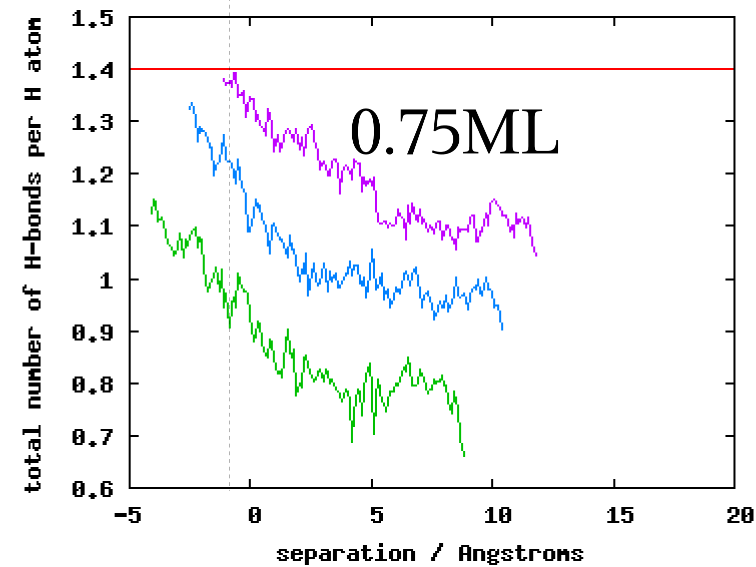

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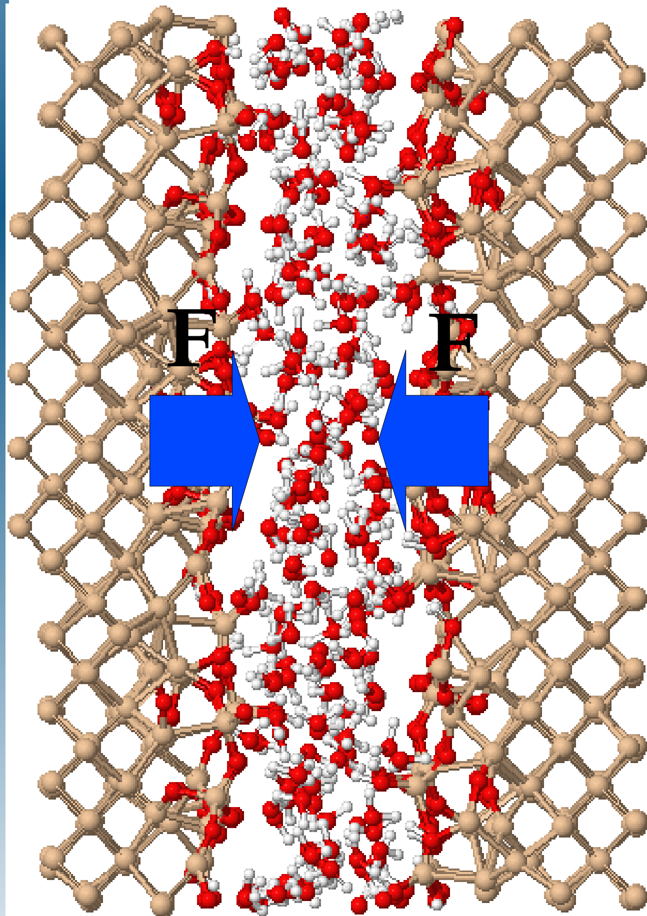

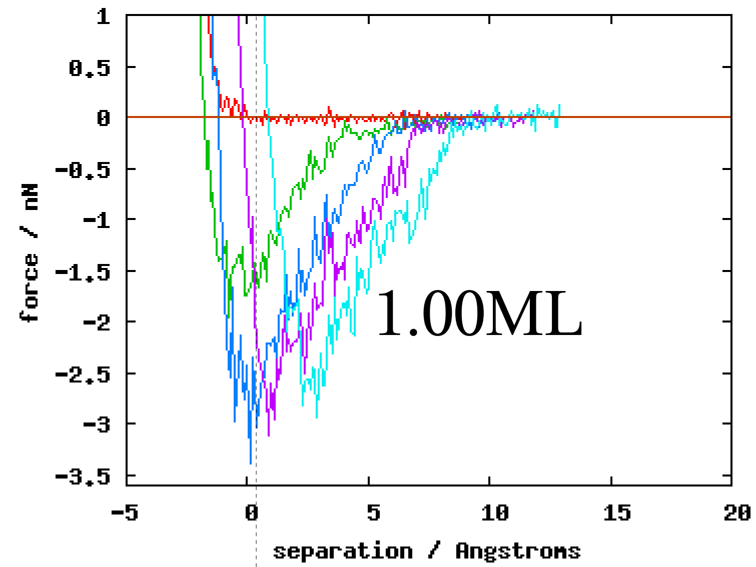

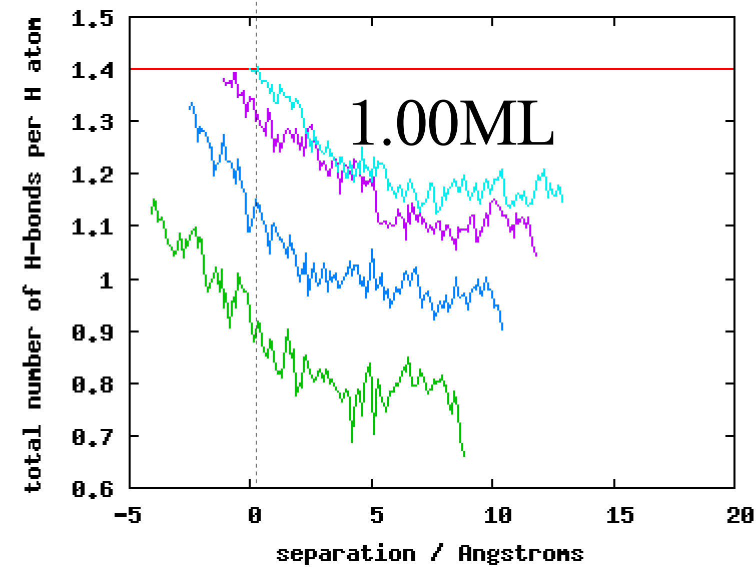

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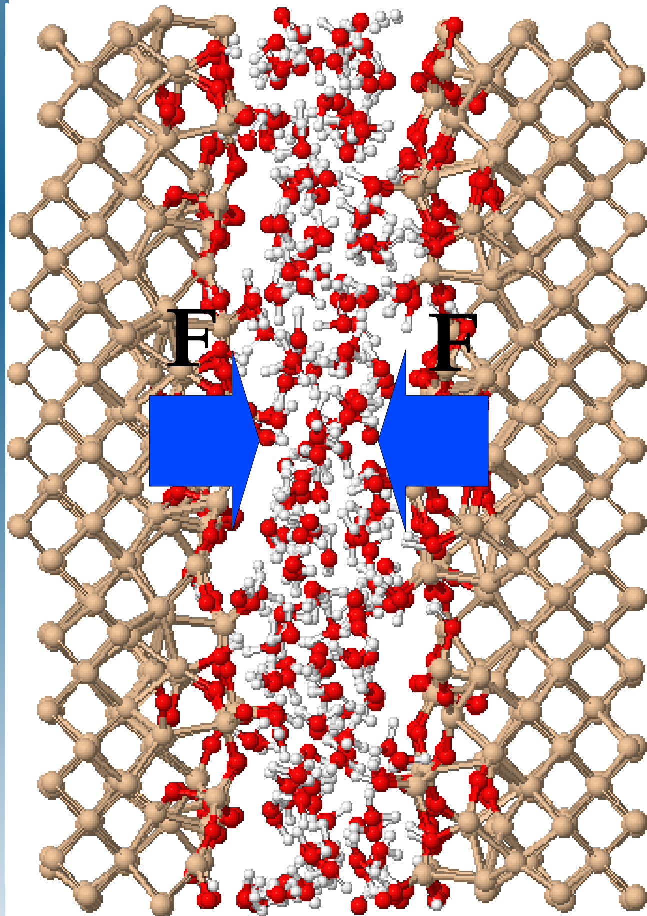
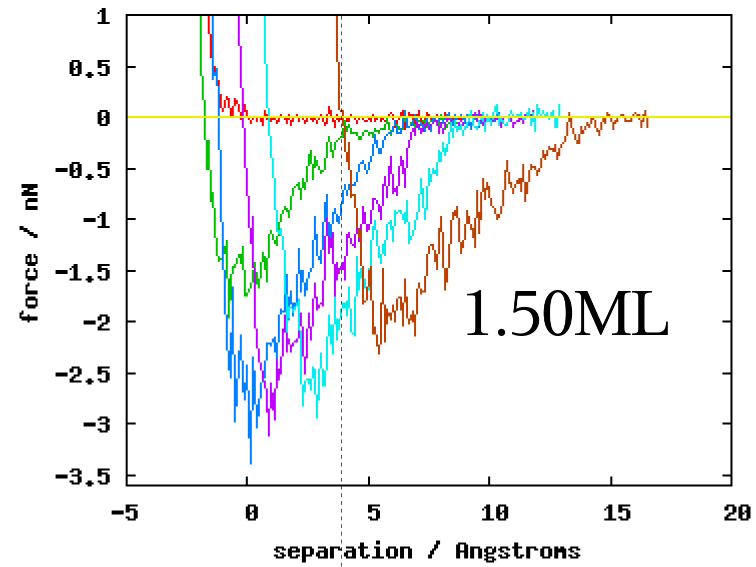
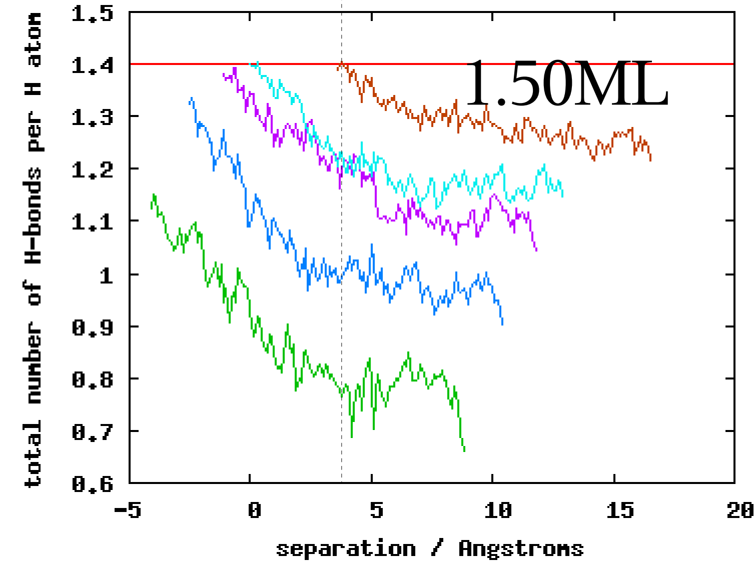
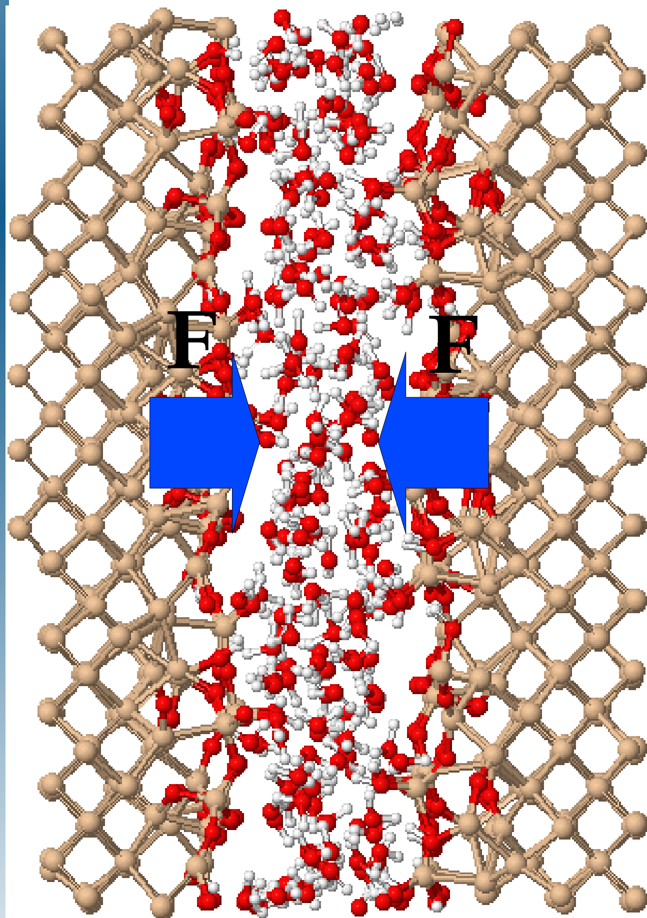
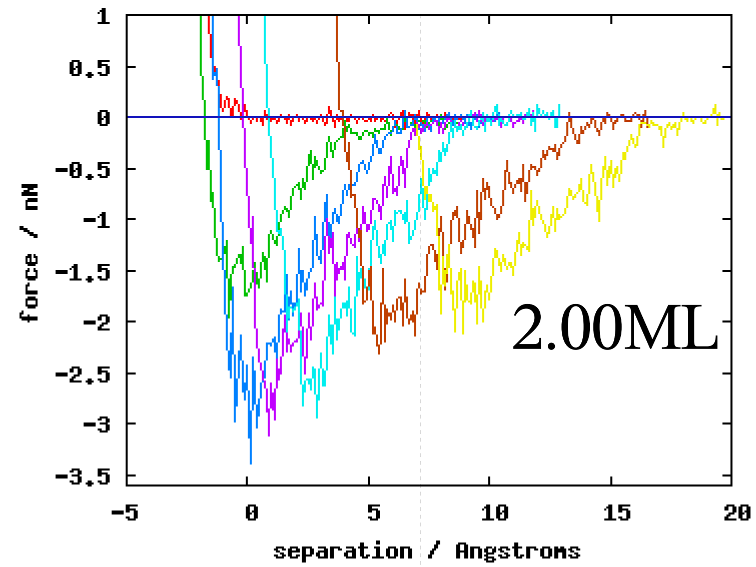


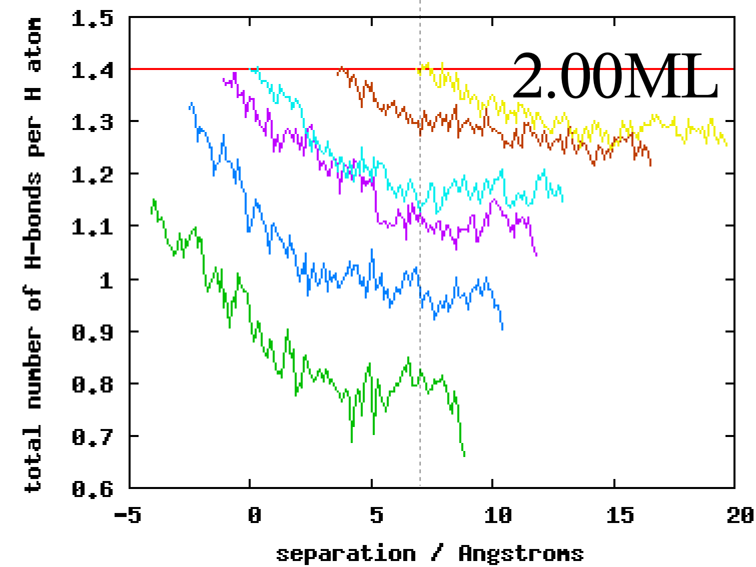




Wafer bonding







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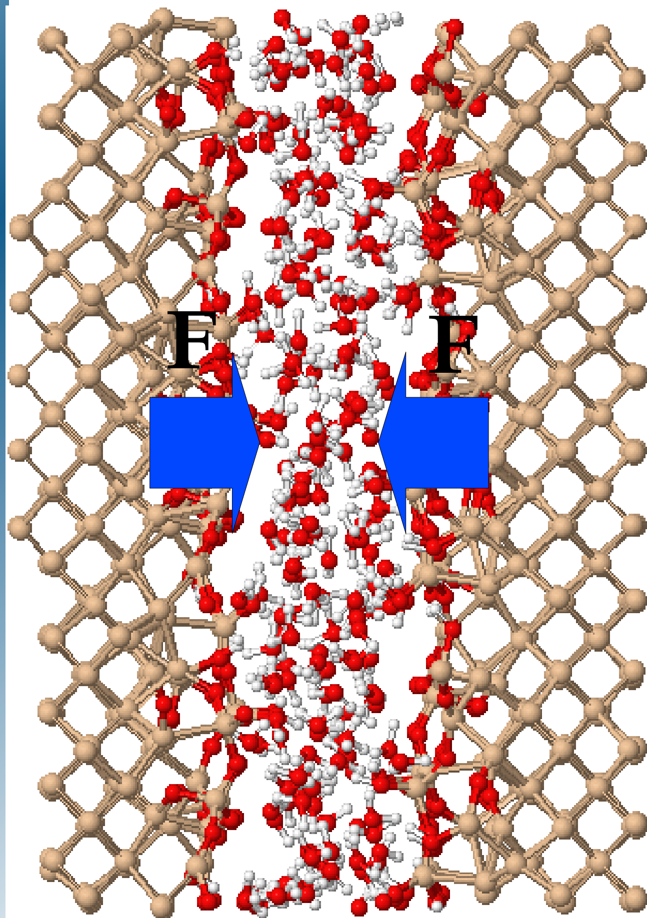

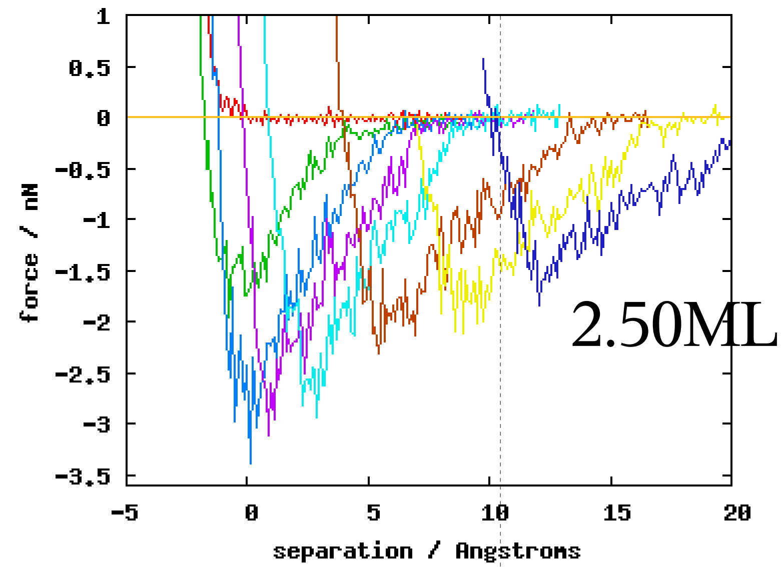

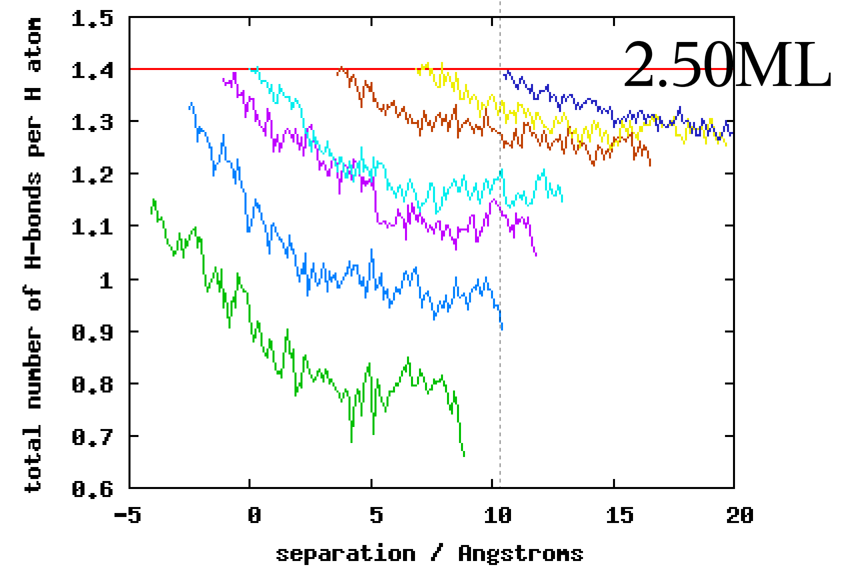

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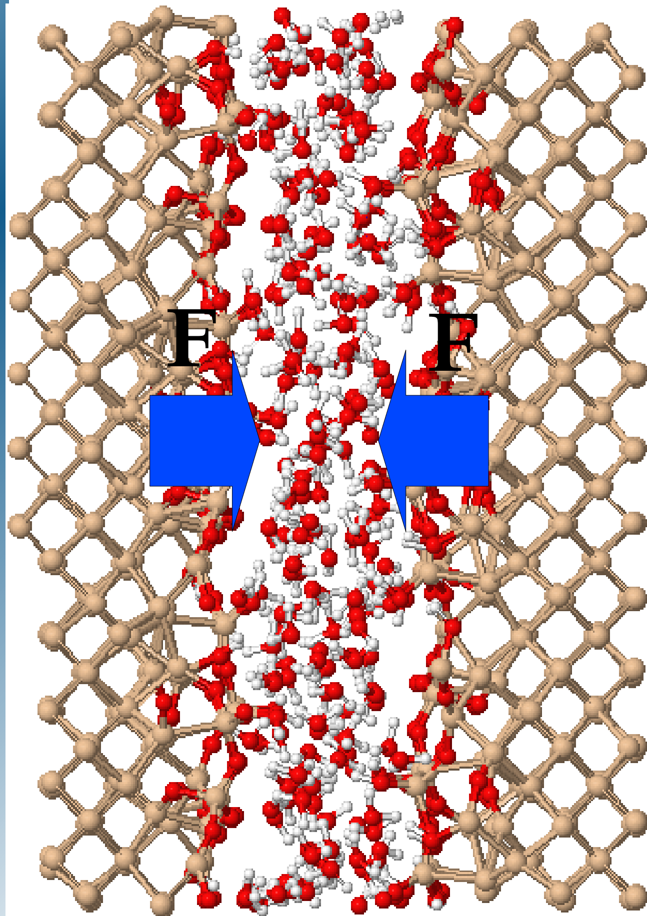
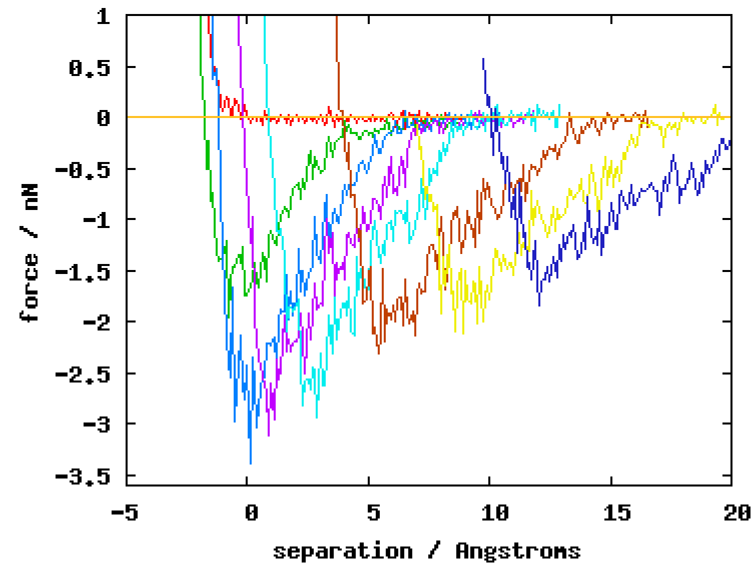
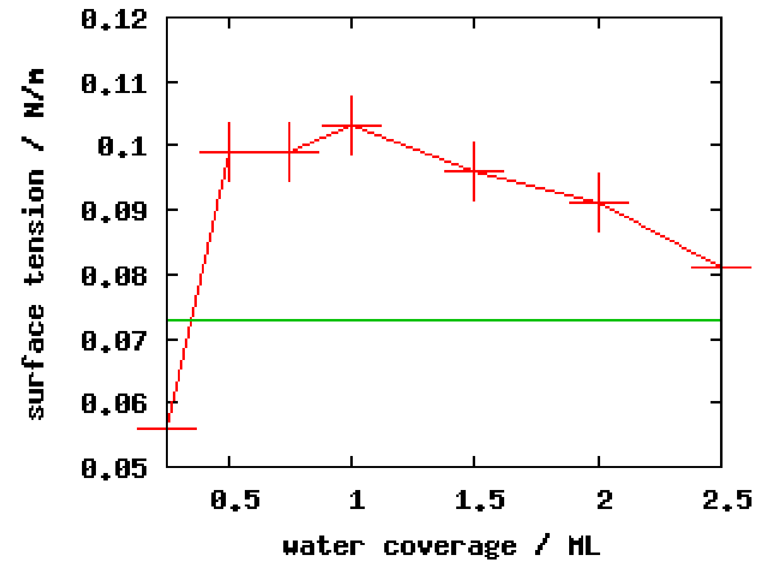
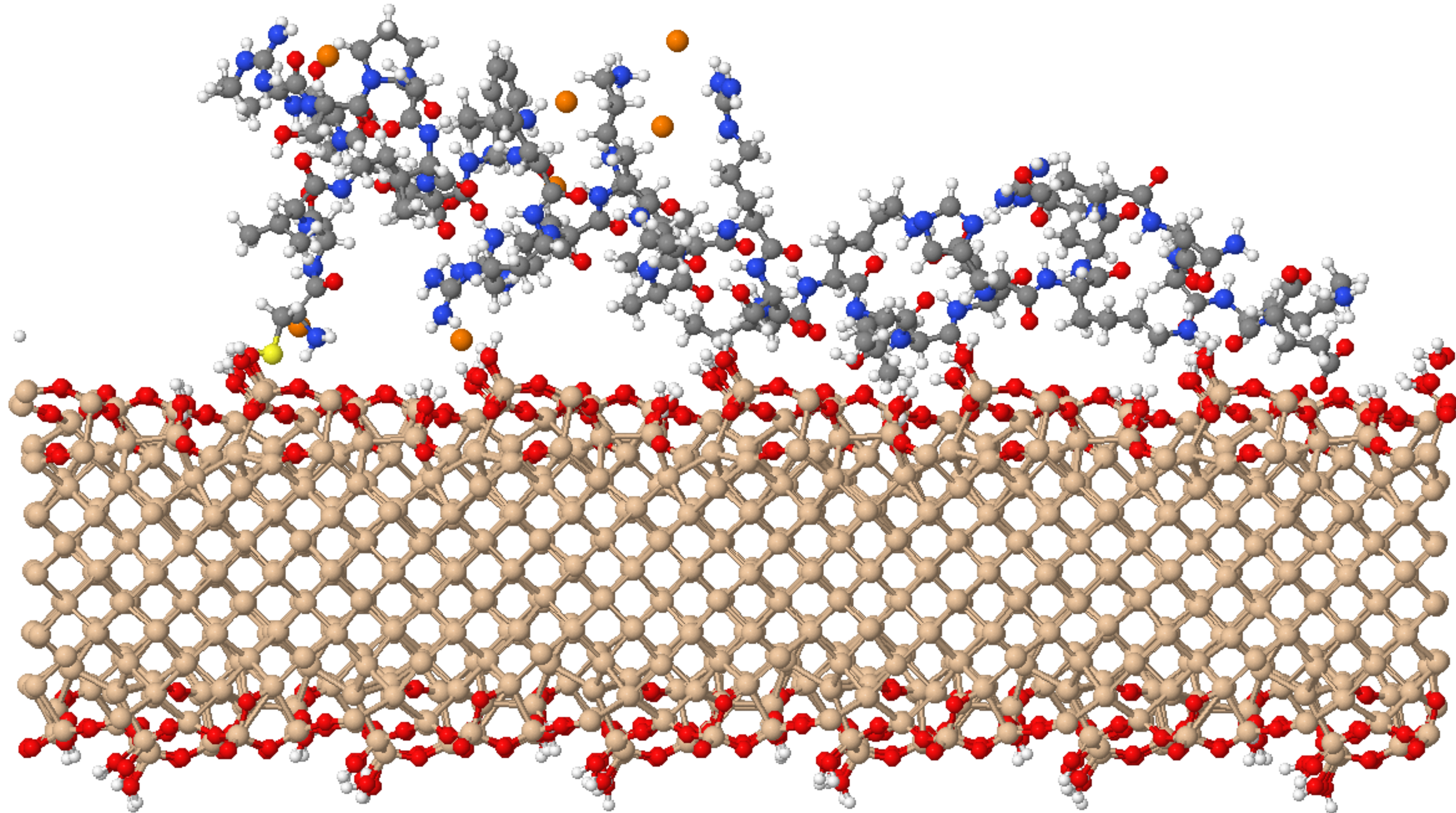






Binding to the NC1 Domain of collagen XIV

- Cells bind to implanted artificial surfaces via extra-cellular matrix proteins, such as collagen



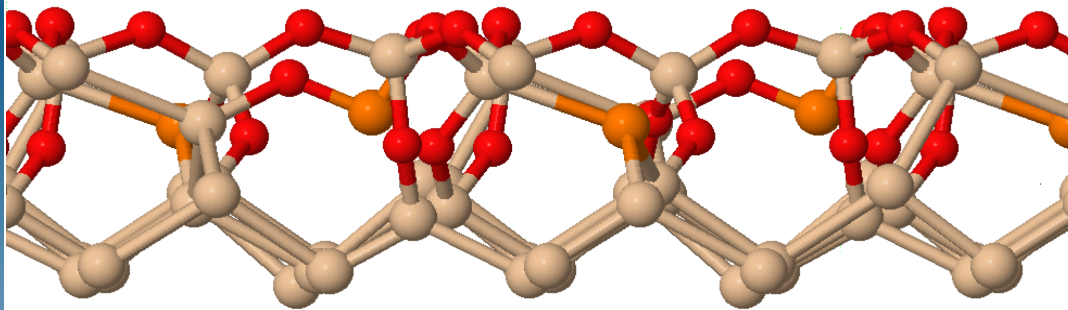
Conclusions

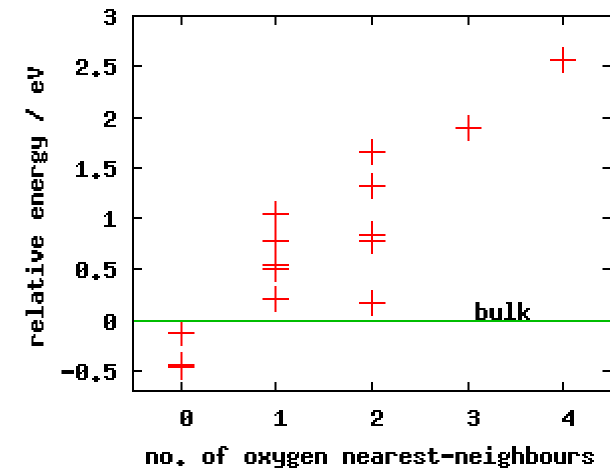
- Classical force field developed that reproduces the structure, charge distribution and tensile stress of the Si hydroxylated native oxide
- Used to simulate room temperature hydrogen bonding between Si wafers
- Future work: continue study of effects of surface chemistry on protein binding to the model Si surface

Impurity segregation

- Do impurities affect the surface electrostatics?

Phosphorous:





Boron: