Atomistic simulations of thermal transport across the solid/liquid interface

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3. **Thermal transport across a nanostructured interface**
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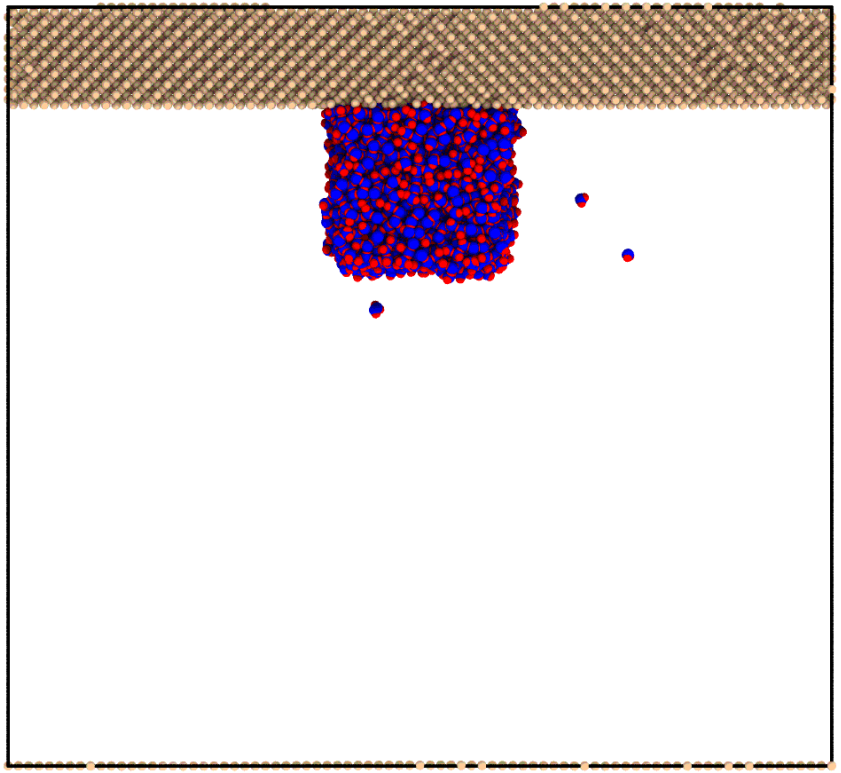
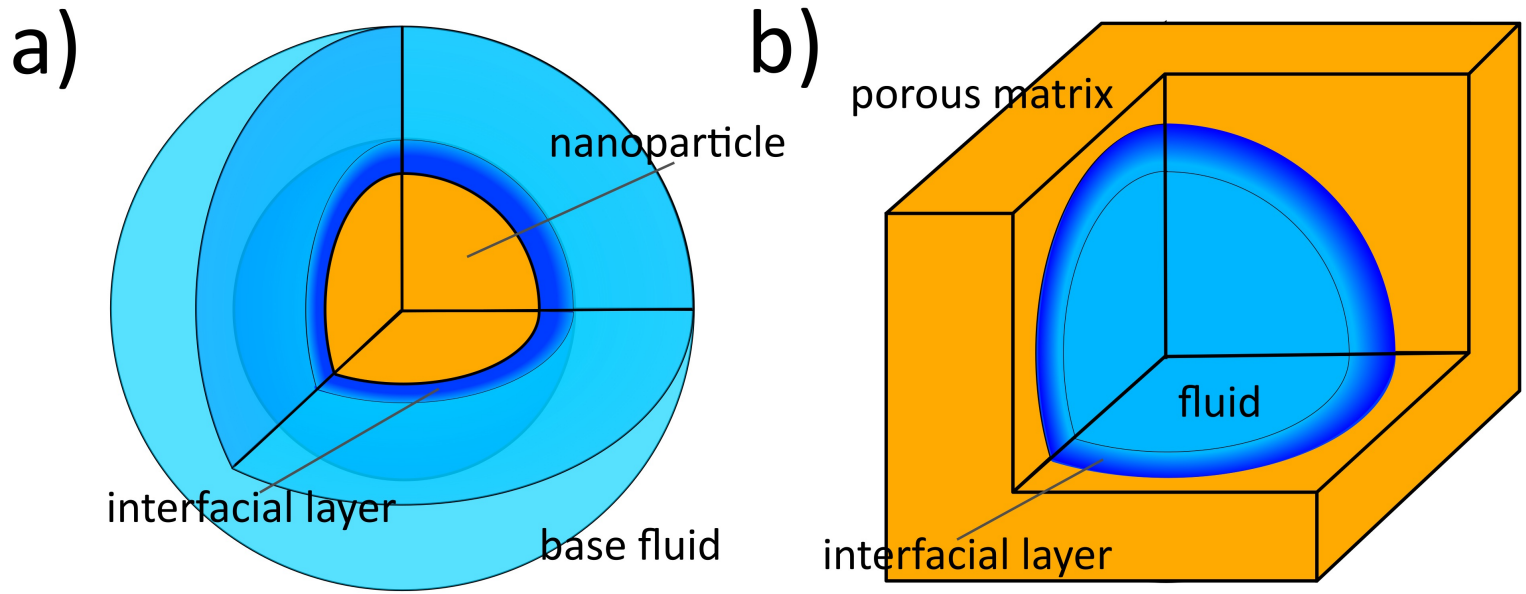
4. **Conclusions**



Motivation



nanofluids

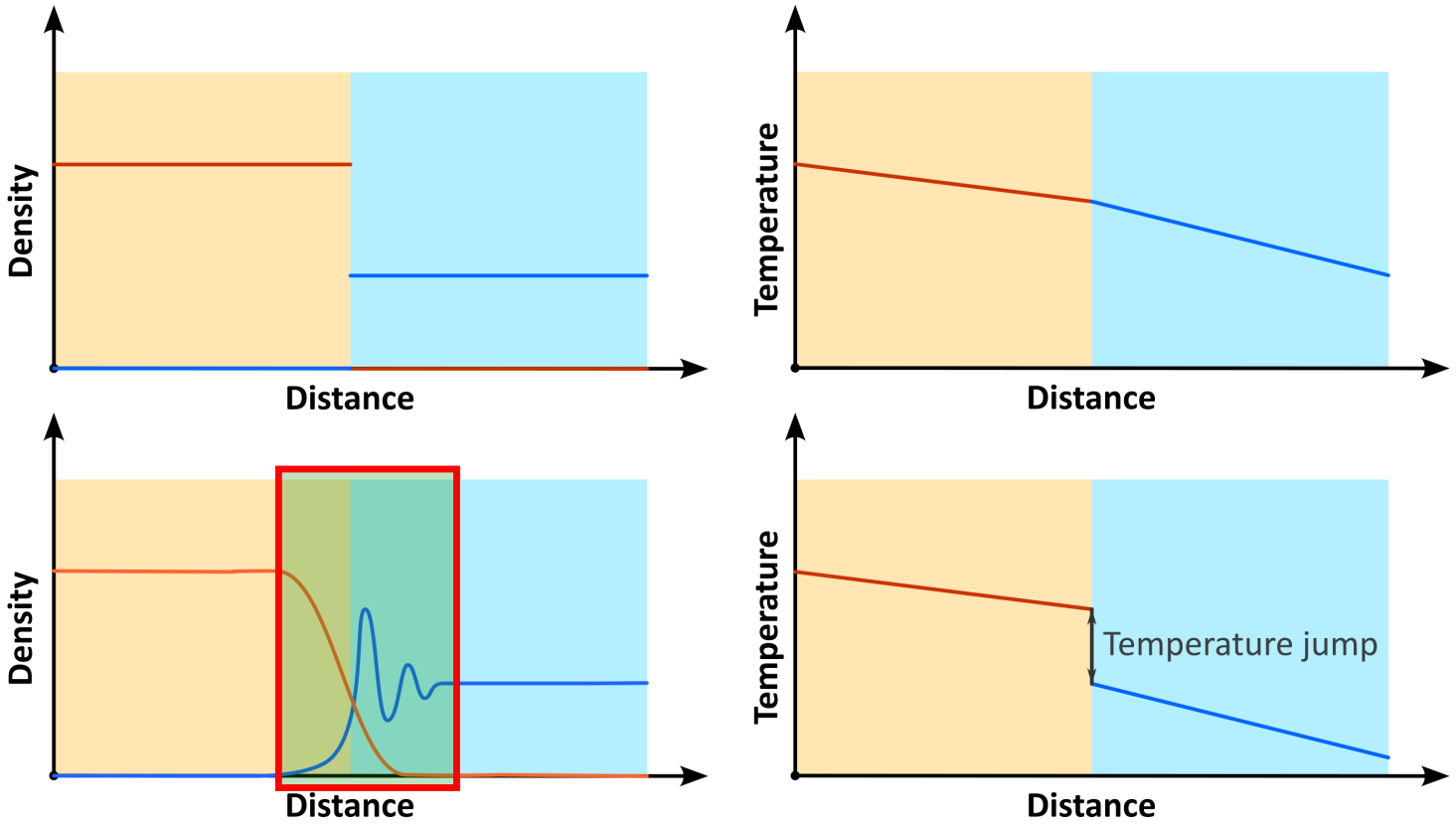
nanoporous matrix

Thermal transport properties of the systems with a significant solid-liquid interface are sensitive to the interfacial thermal transport

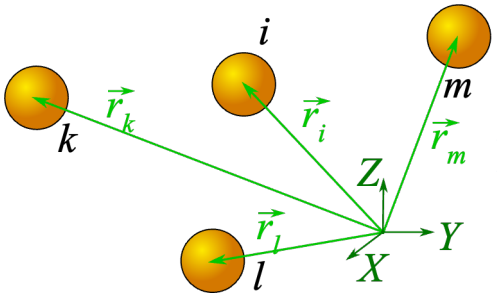
Motivation

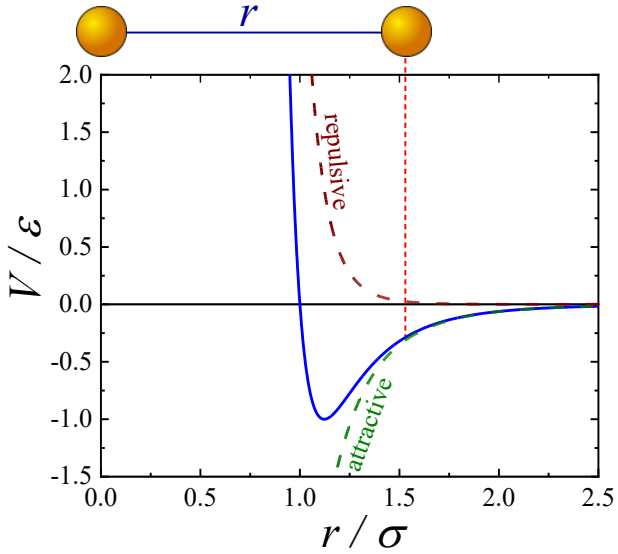
Macroscale

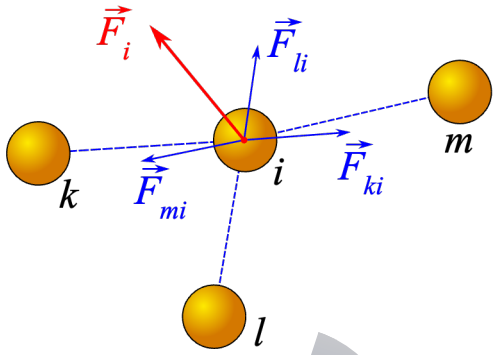
Nanoscale



Molecular dynamics





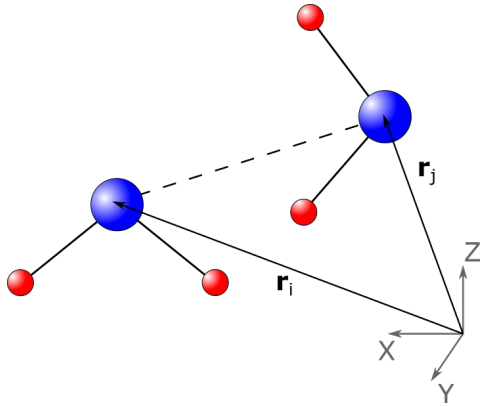


$$m_i \overrightarrow{a_i} = \sum_{j \neq i}^{N} \vec{F}_{ij} + \vec{F}_{i\,ext}$$

Evolution of the system with respect of classical Newton law of motion

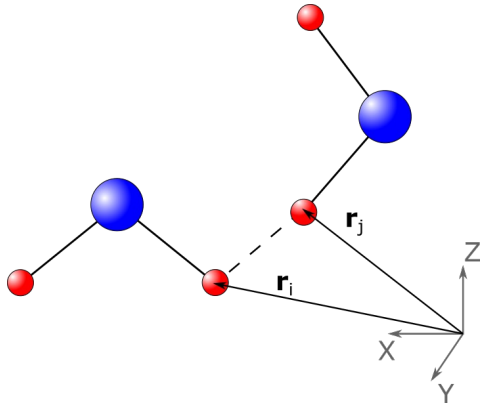
Water model

O-O



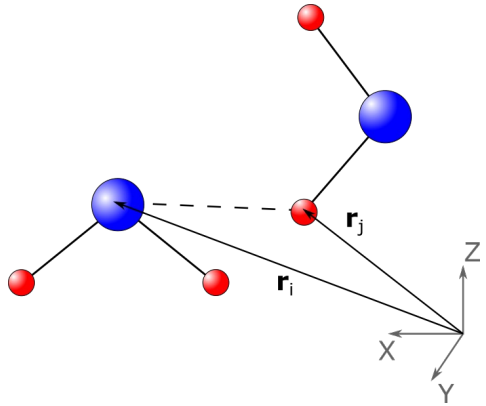
$$V_{O-O} = \frac{1}{4\pi\varepsilon_1\varepsilon_0}\frac{(q_O)^2}{|\vec{r}_i - \vec{r}_j|} + 4\varepsilon\left(\left(\frac{\sigma}{|\vec{r}_i - \vec{r}_j|}\right)^{12} - \left(\frac{\sigma}{|\vec{r}_i - \vec{r}_j|}\right)^{6}\right)$$

H-H



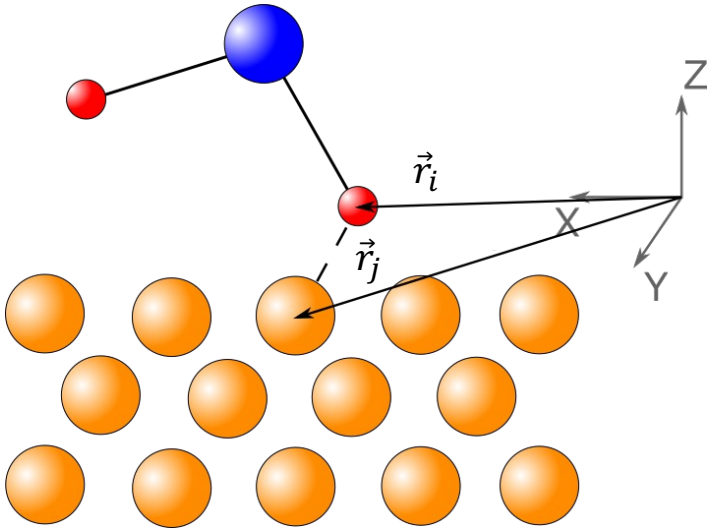
$$V_{H-H} = \frac{1}{4\pi\varepsilon_1\varepsilon_0}\frac{(q_H)^2}{|\vec{r}_i - \vec{r}_j|}$$

O-H

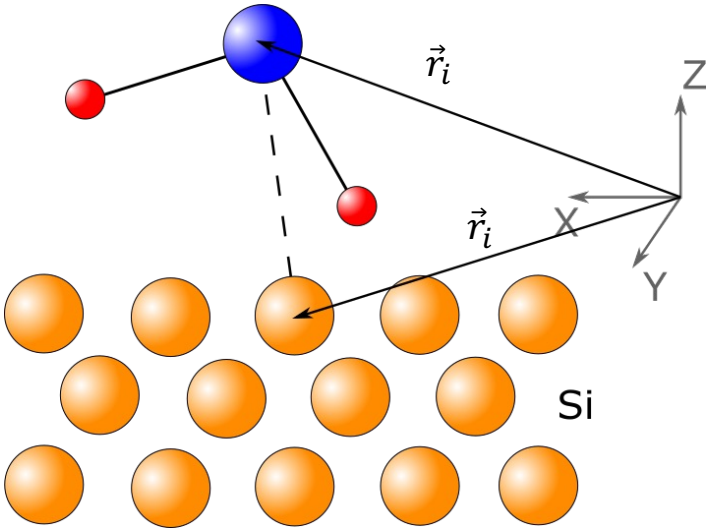


$$V_{O-H} = \frac{1}{4\pi\varepsilon_1\varepsilon_0}\frac{q_O q_H}{|\vec{r}_i - \vec{r}_j|}$$

Solid/liquid interactions

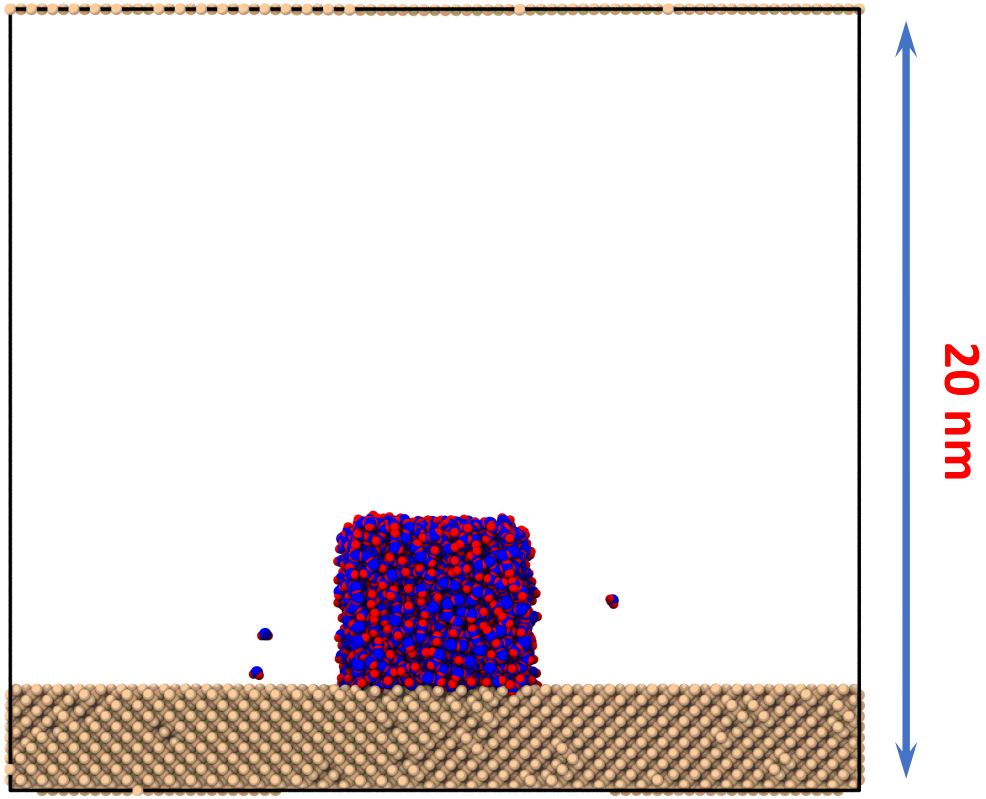


$$V_{O-Si} = 0$$



$$V_{O-Si} = 4\varepsilon_{O-Si}\left(\left(\frac{\sigma_{O-Si}}{r}\right)^{12} - \left(\frac{\sigma_{O-Si}}{r}\right)^{6}\right)$$

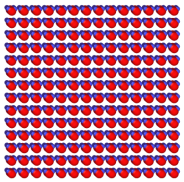
Wetting phenomena

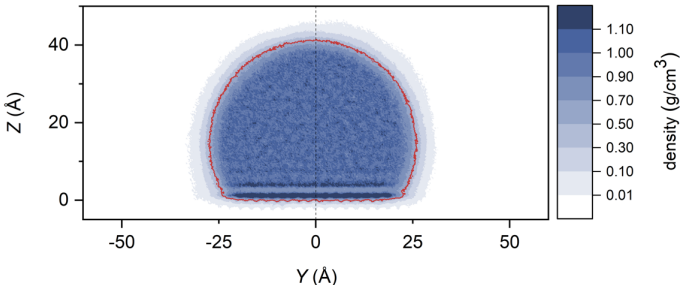


32 000 of silicon atoms
6820 water molecules

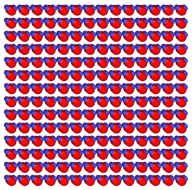
Wetting phenomena

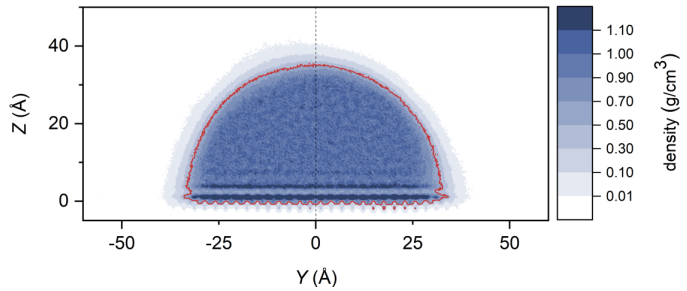
$\varepsilon_{O\text{-}Si}$ = 10 meV



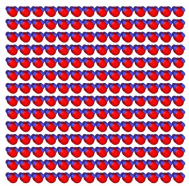


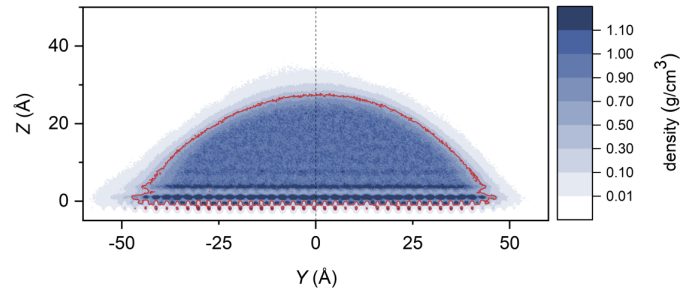
$\varepsilon_{O\text{-}Si}$ = 15 meV



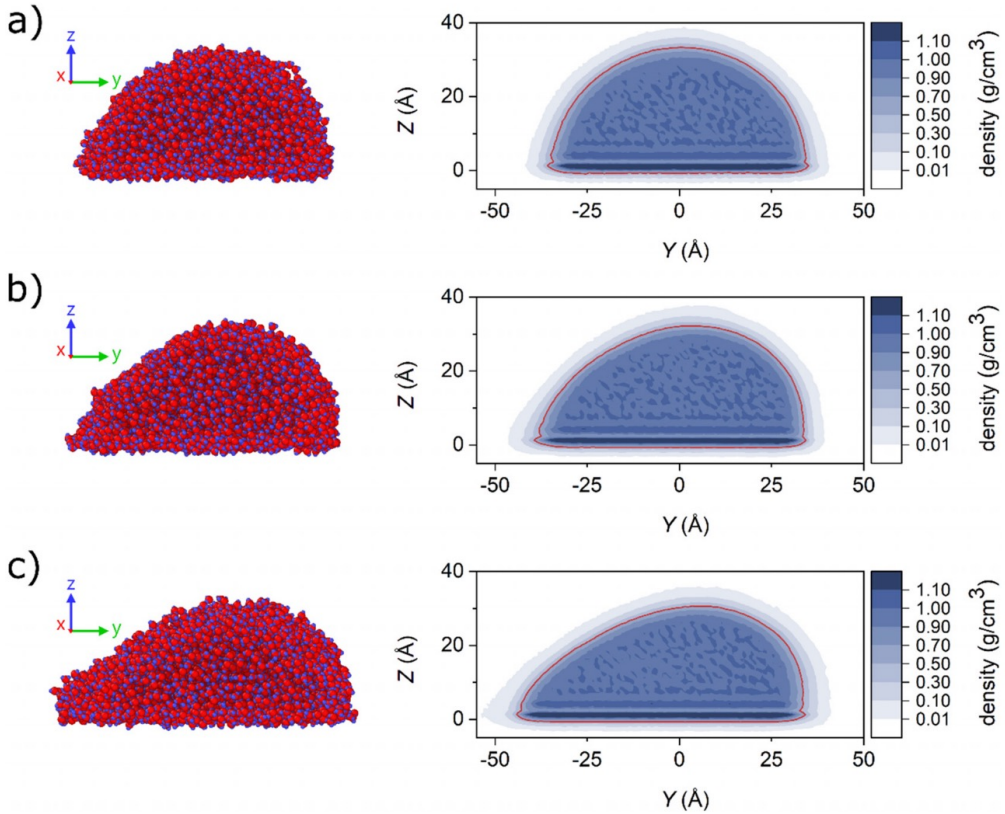


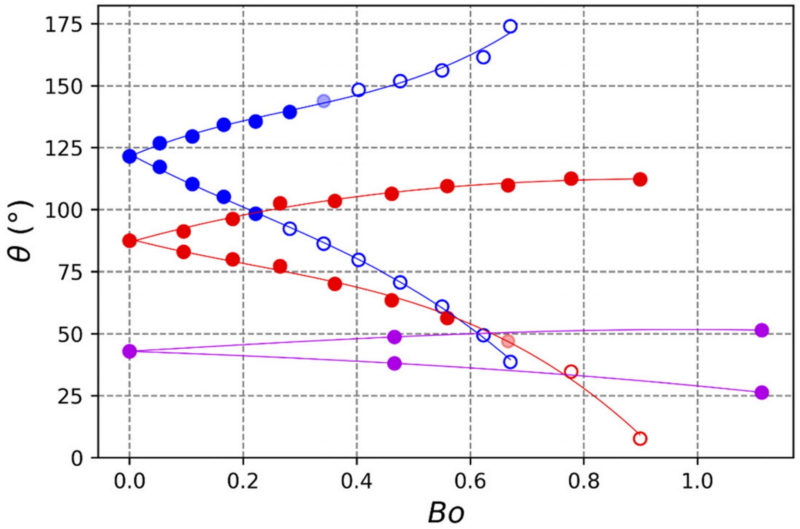
$\varepsilon_{O\text{-}Si}$ = 21 meV





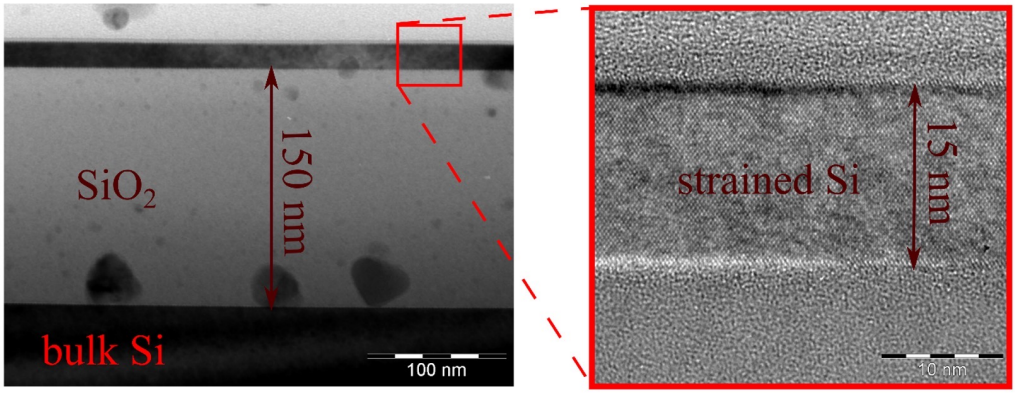
Wetting phenomena

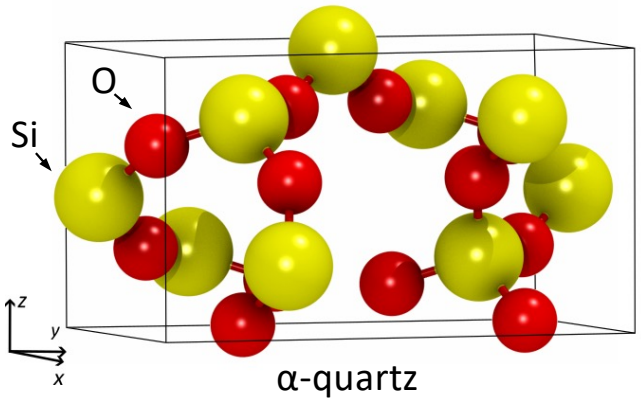




Mandrolko, V., …, & Isaiev, M. (2024). Features of the contact angle hysteresis at the nanoscale: A molecular dynamics insight. *Physics of Fluids*, *36*(5), 052012.

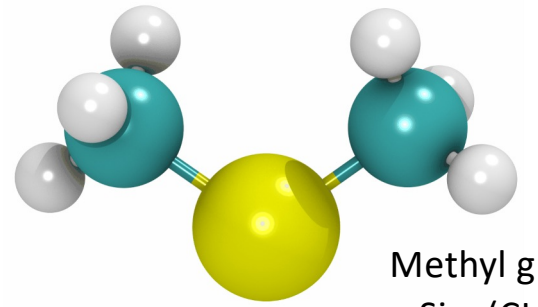
More complex interface



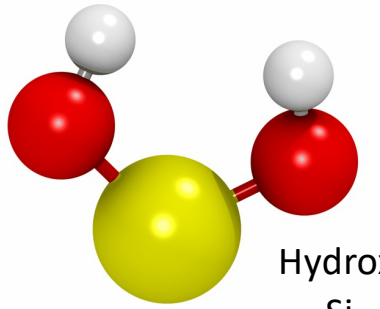


α-quartz

Functionalization

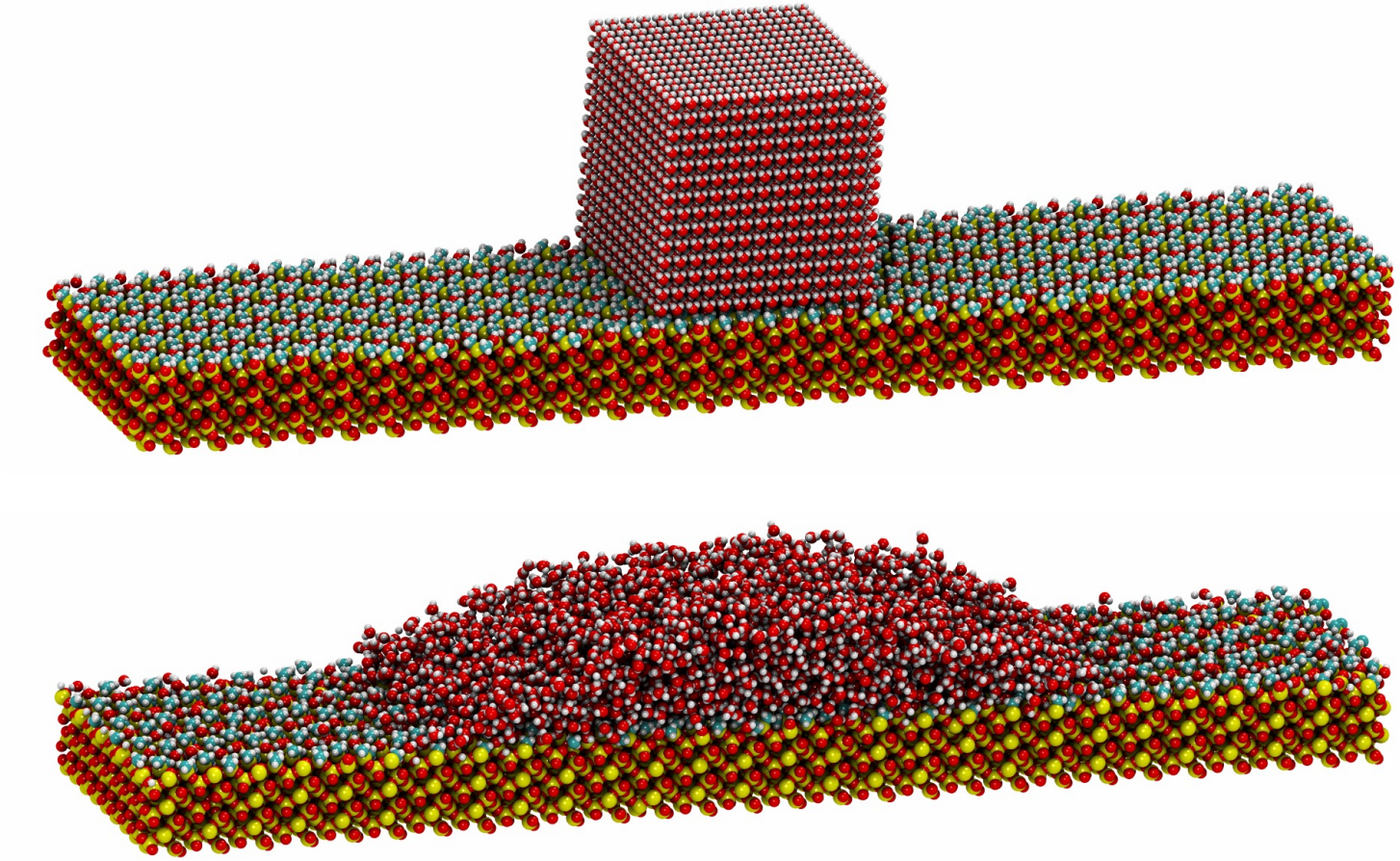


Methyl group
$Si - (CH_3)_2$
+hydrophobicity

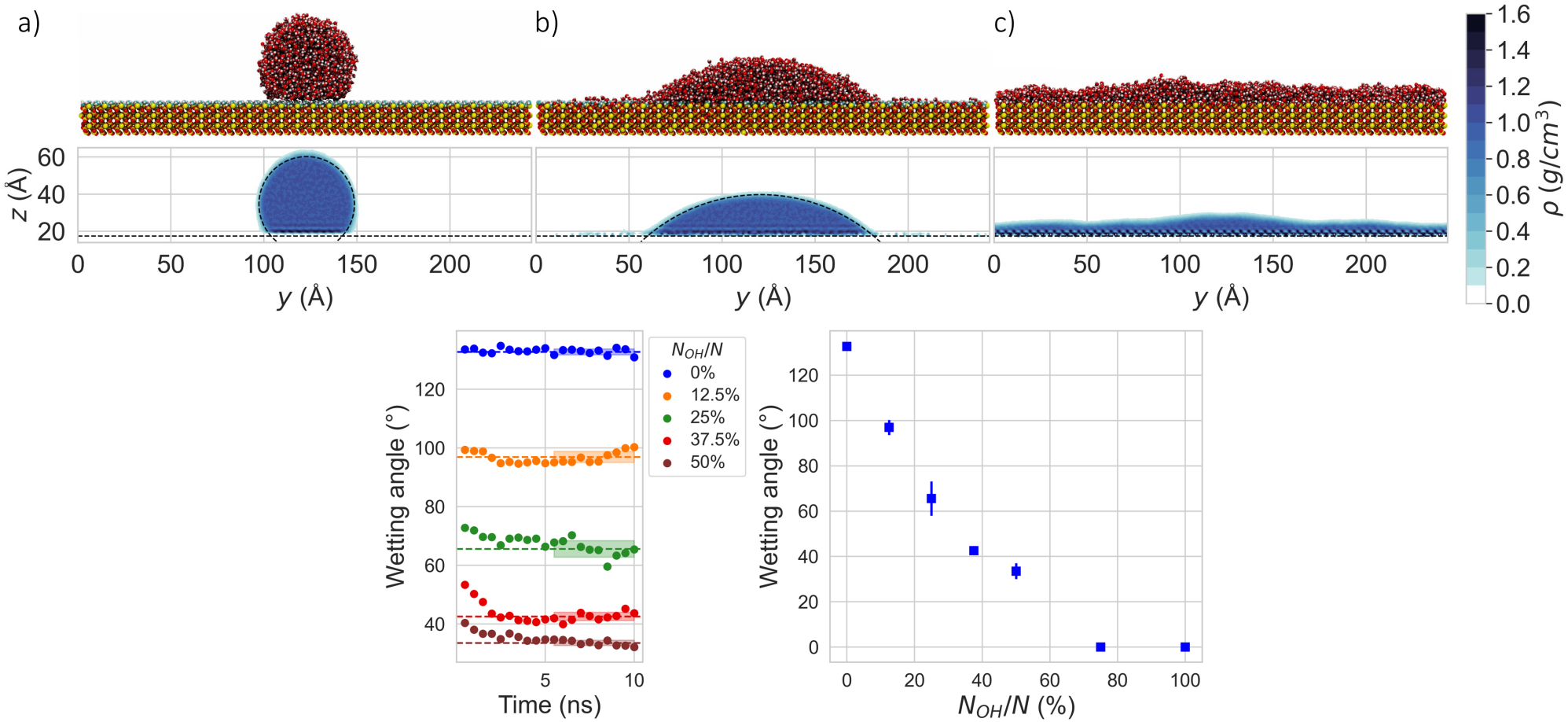


Hydroxyl group
$Si - (OH)_2$
+hydrophilicity

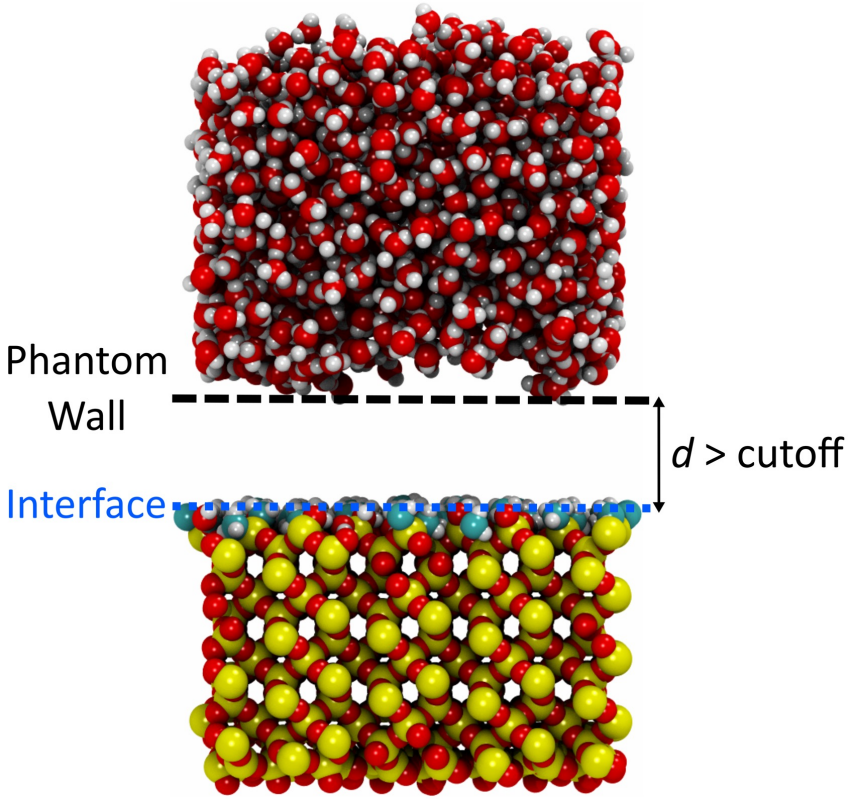
Functionalised silica interface

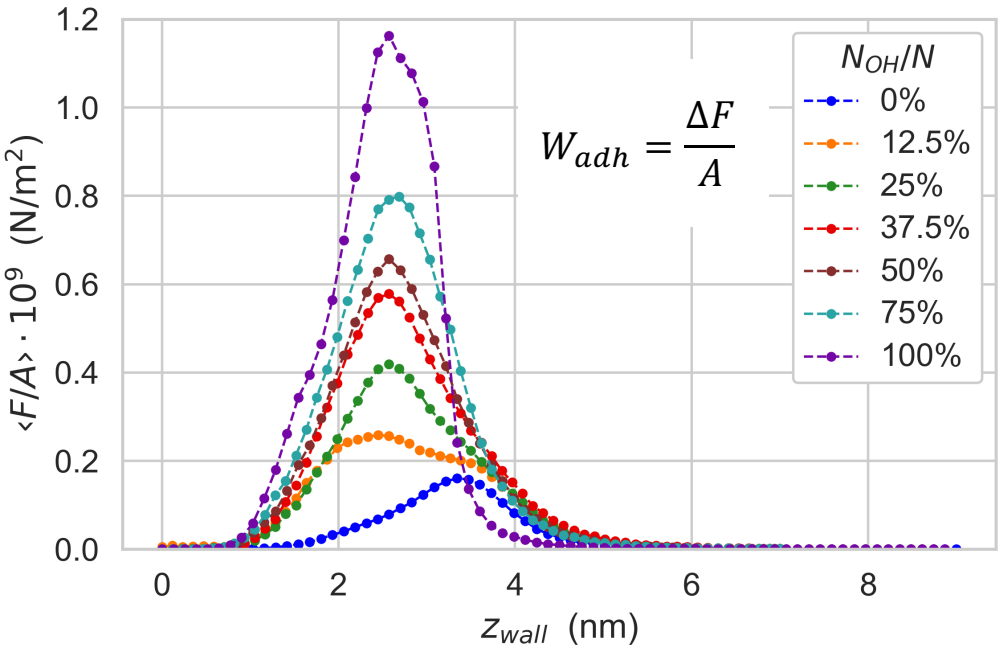


Functionalised silica interface

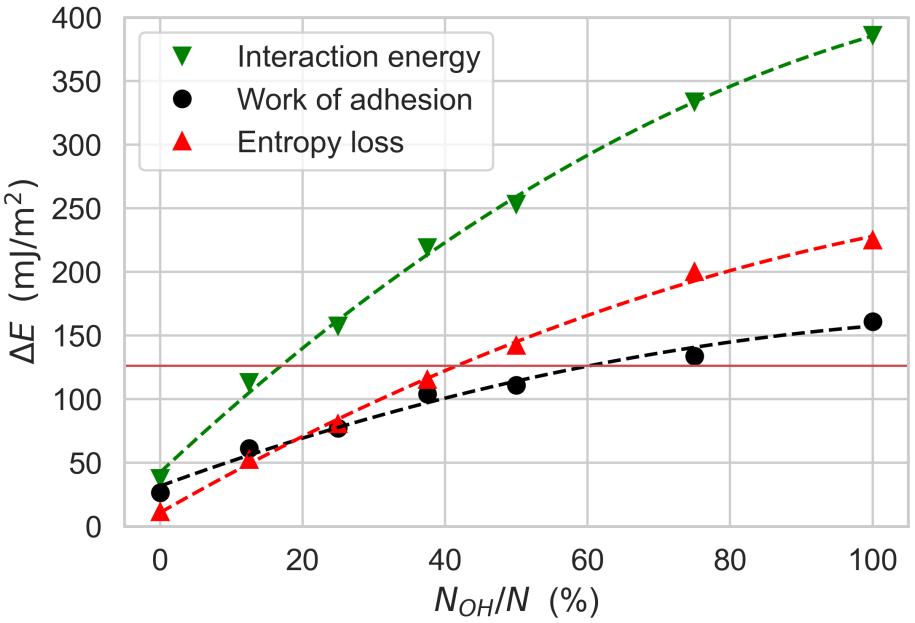


Work of adhesion





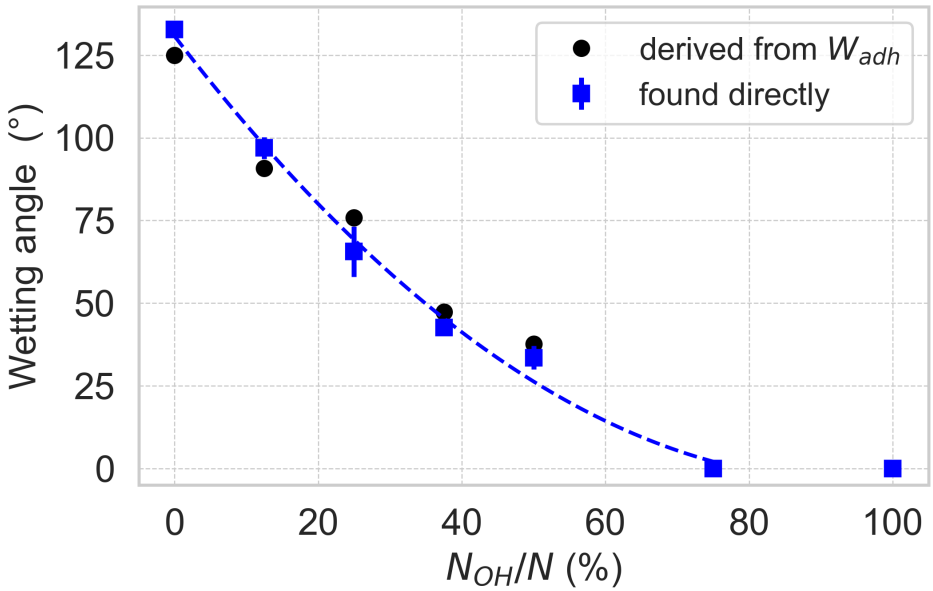
Work of adhesion vs contact angle



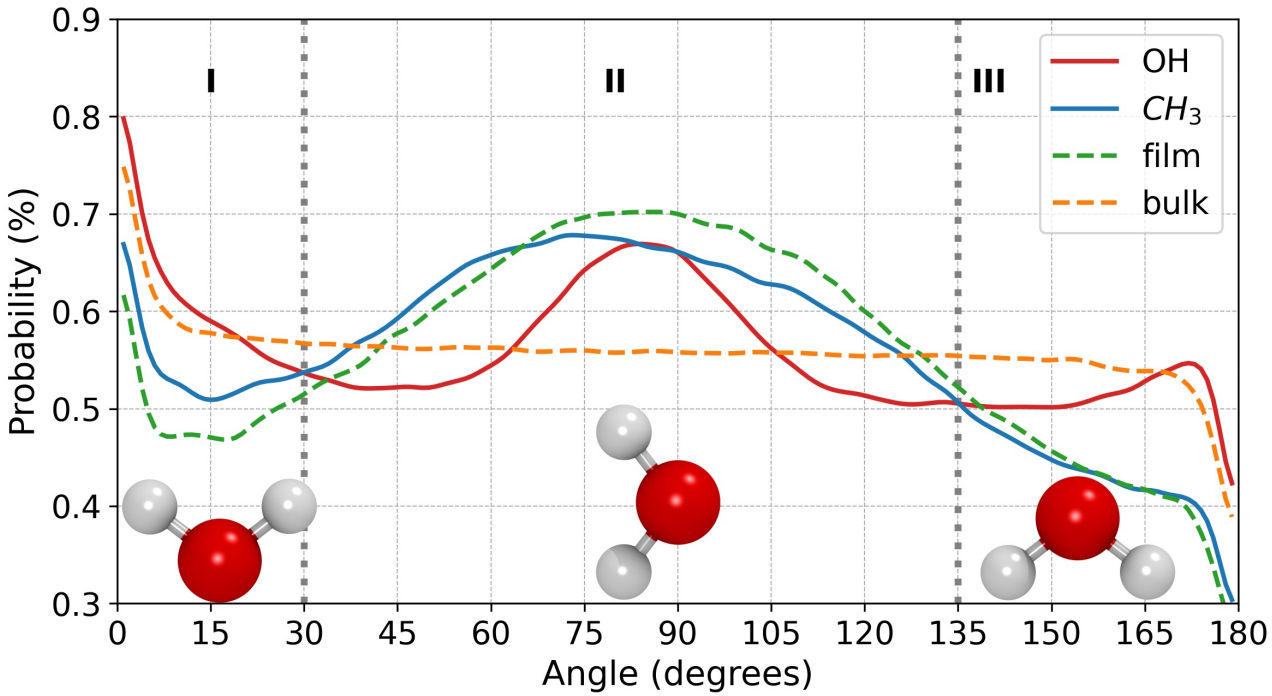
Young-Dupré equation

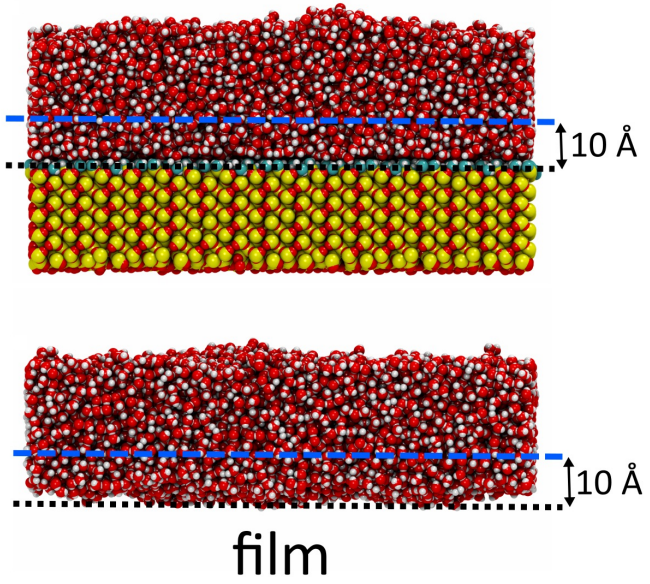
$$W_{adh} = \gamma_{lv}(1 + \cos\theta)$$

Work of adhesion — Surface tension — Wetting angle



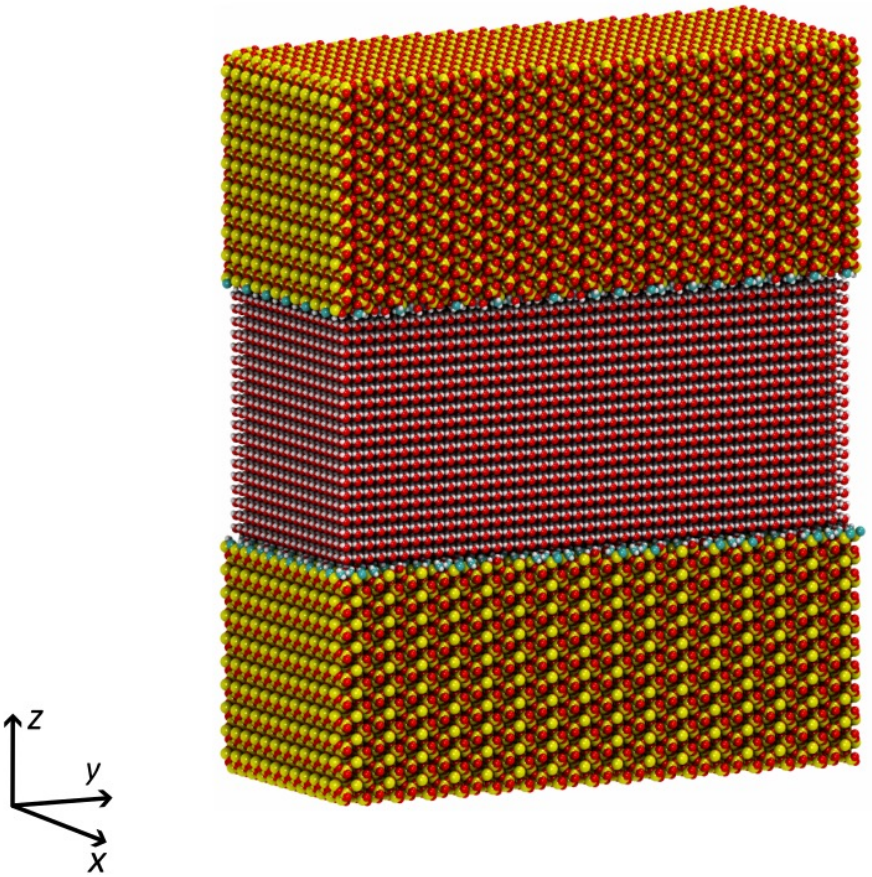
Probability of the water molecules' orientation



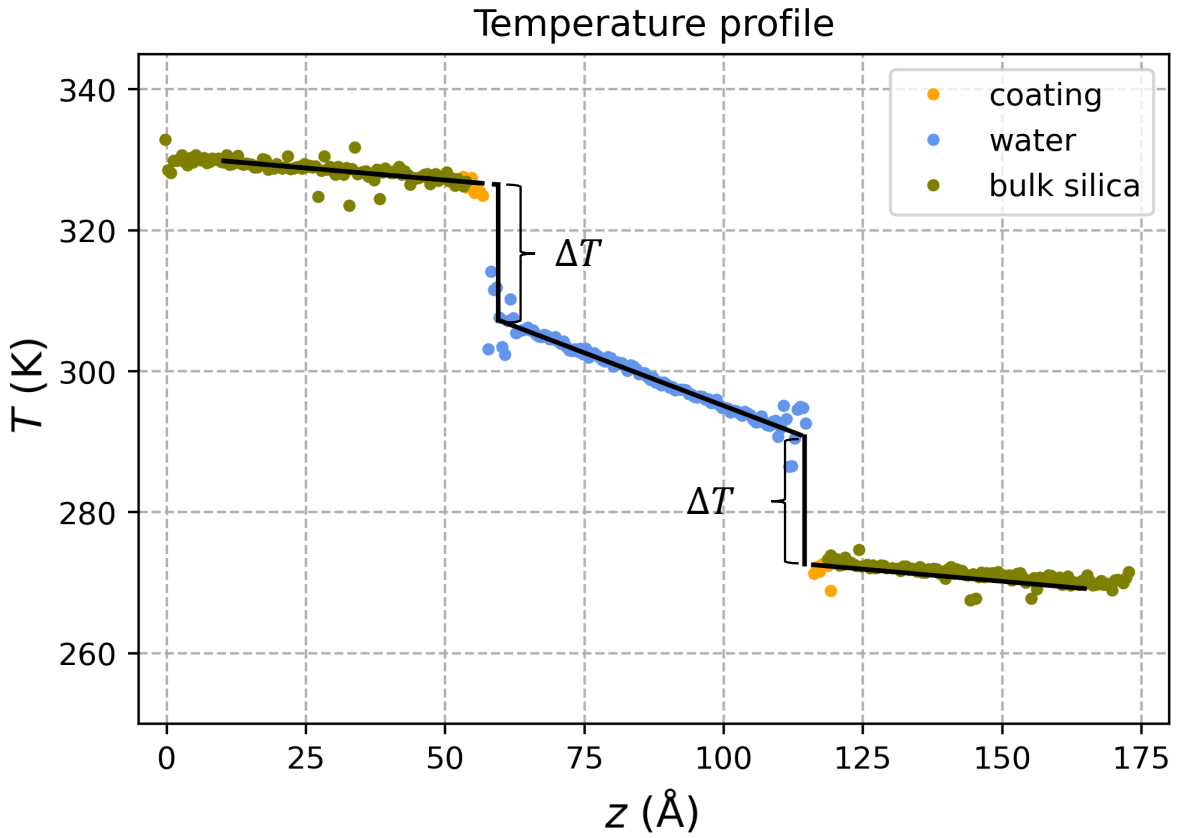


More perpendicular hydrogen bonds are formed for a hydrophilic (OH) surface, facilitating heat transfer

Thermal transport



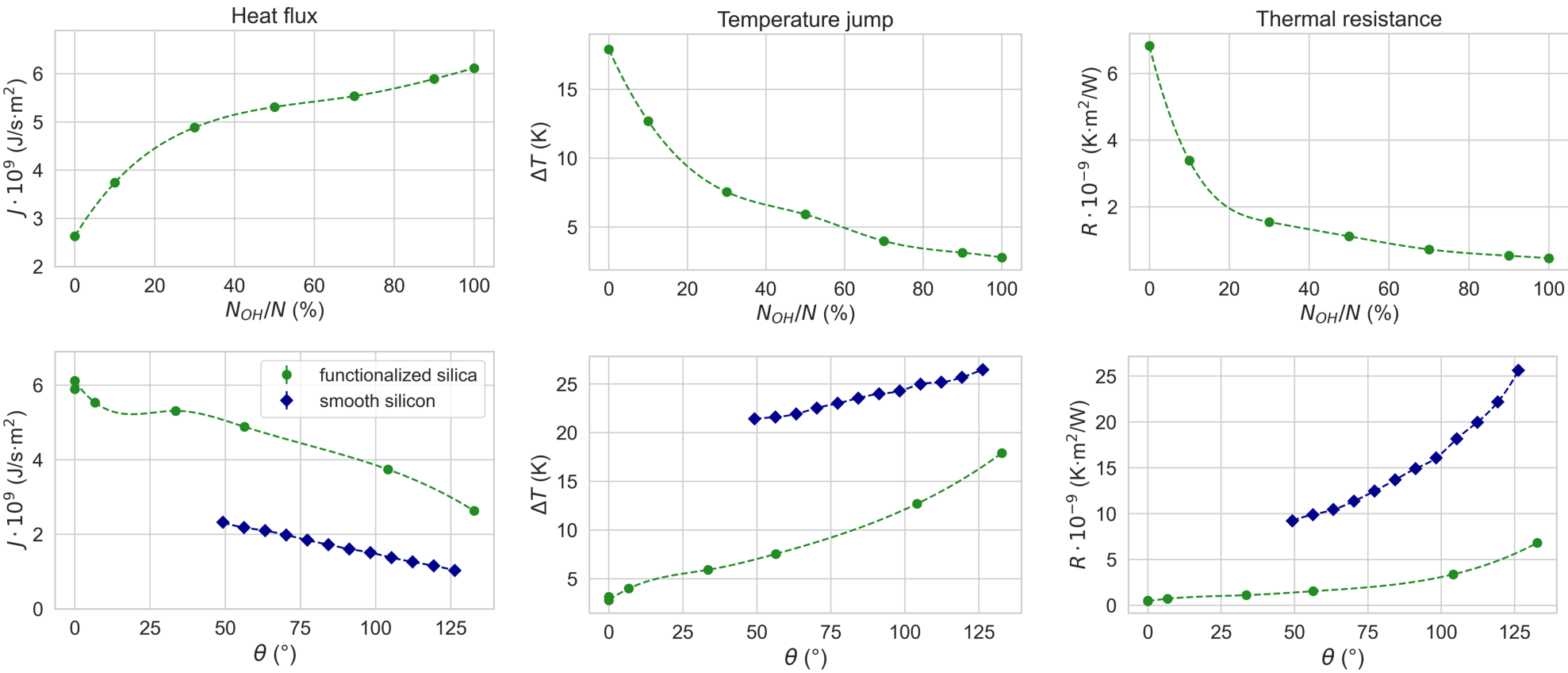
Interfacial thermal resitence



Thermal resistance:

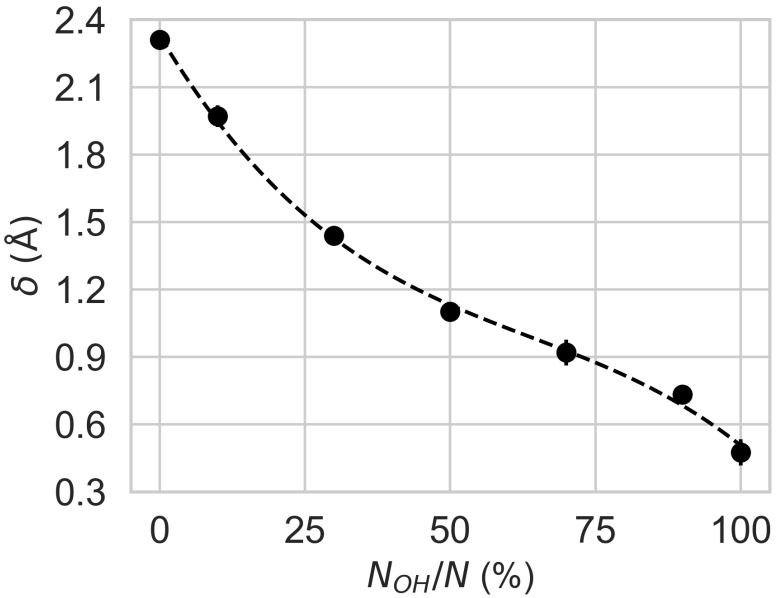
$$R = \frac{\Delta T}{J}$$

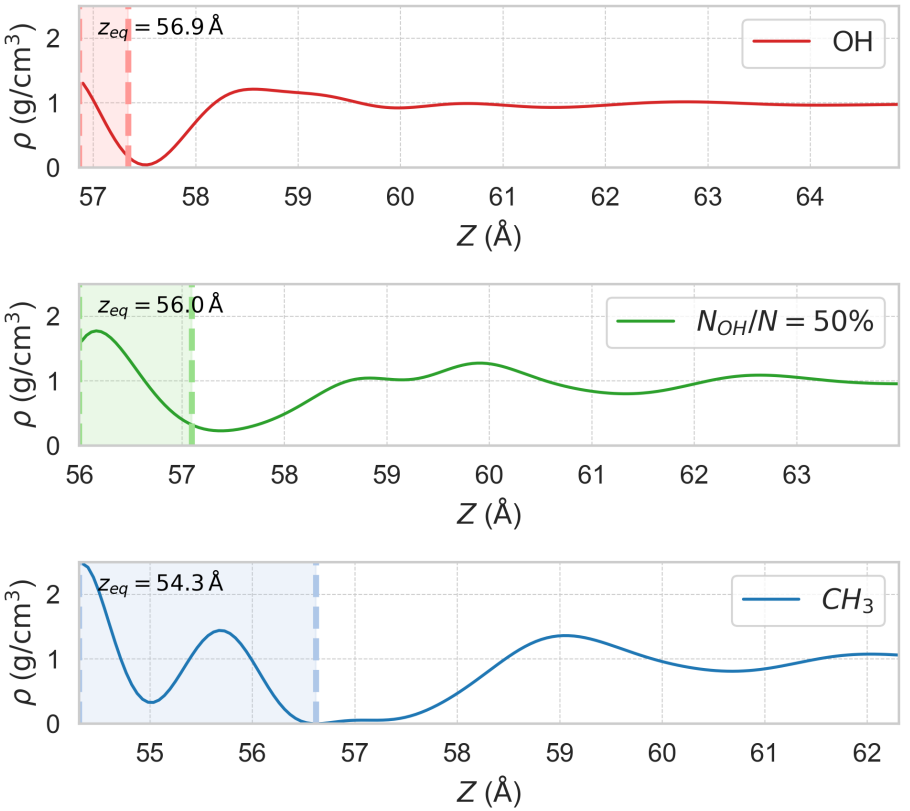
Interfacial thermal resistance



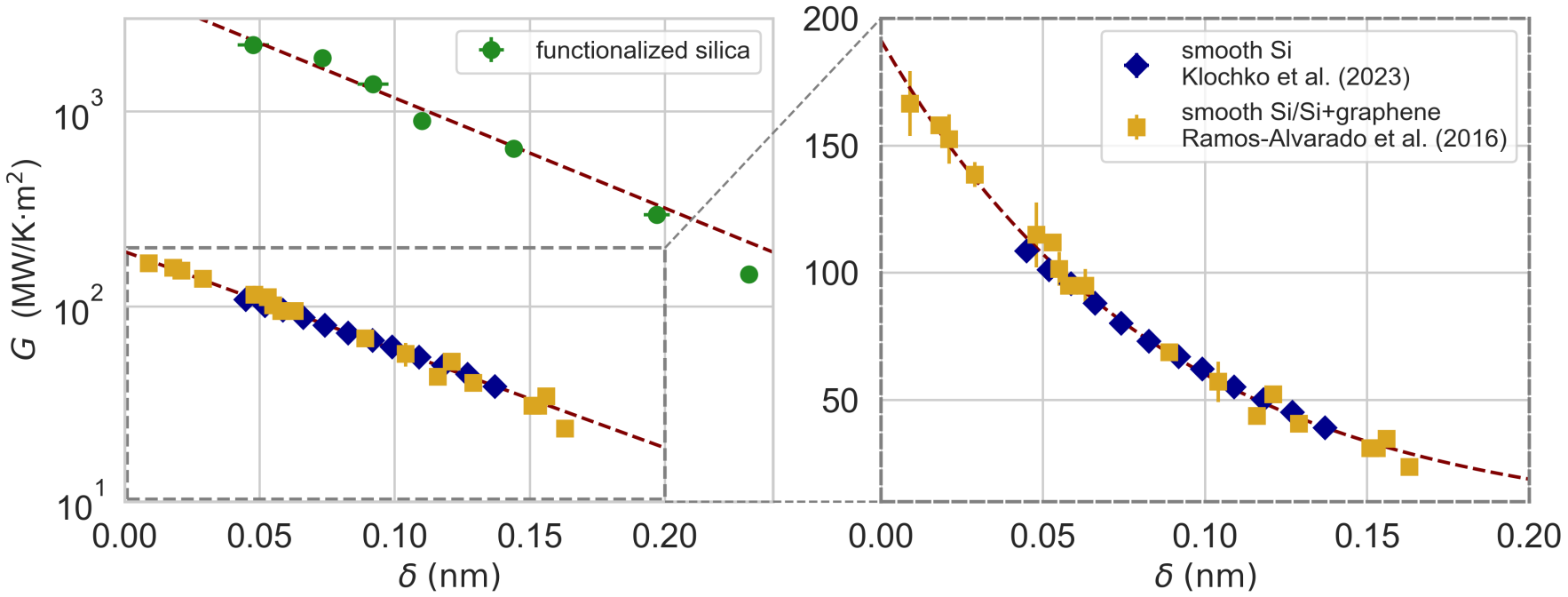
Interfacial thermal resistance

$$\delta = \int_0^{\infty} \left[1 - \frac{\rho_s(z)}{\rho_s^b} - \frac{\rho_l(z)}{\rho_l^b} \right] dz$$

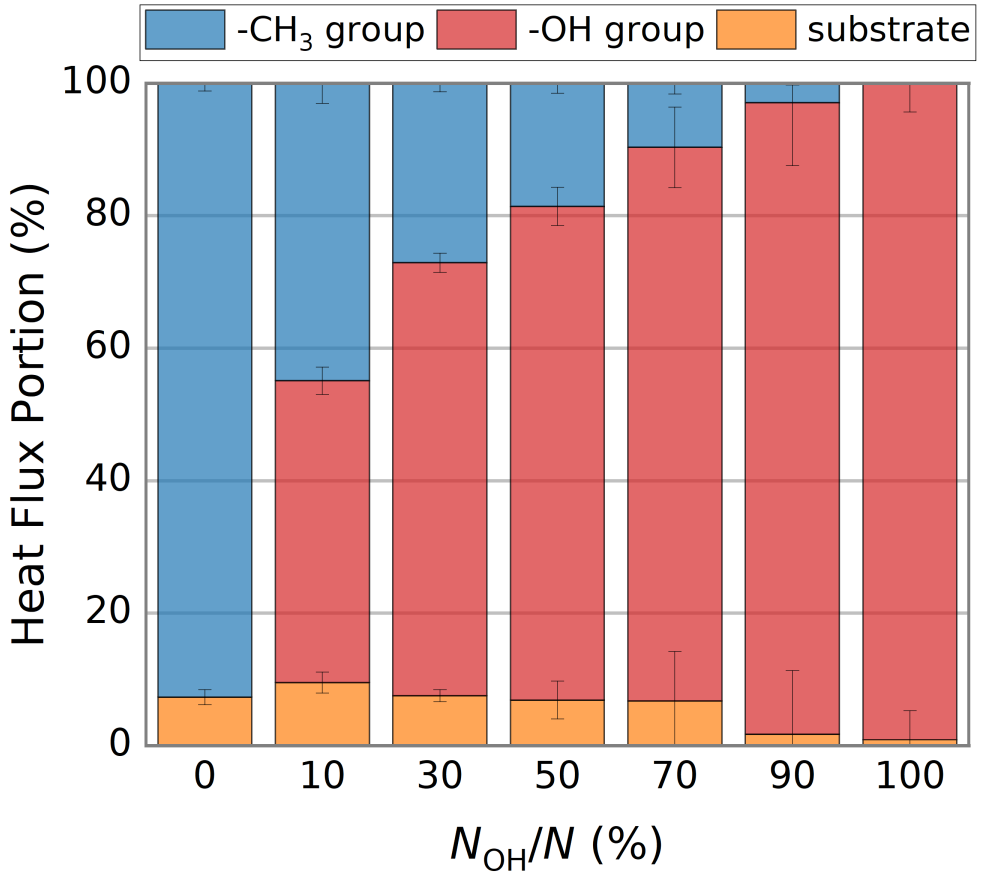




Interfacial thermal resistance

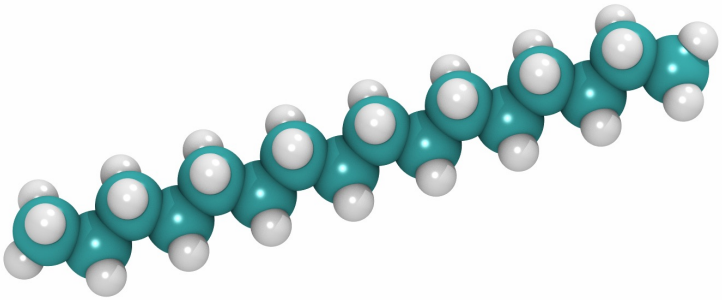


Heat flux decomposition

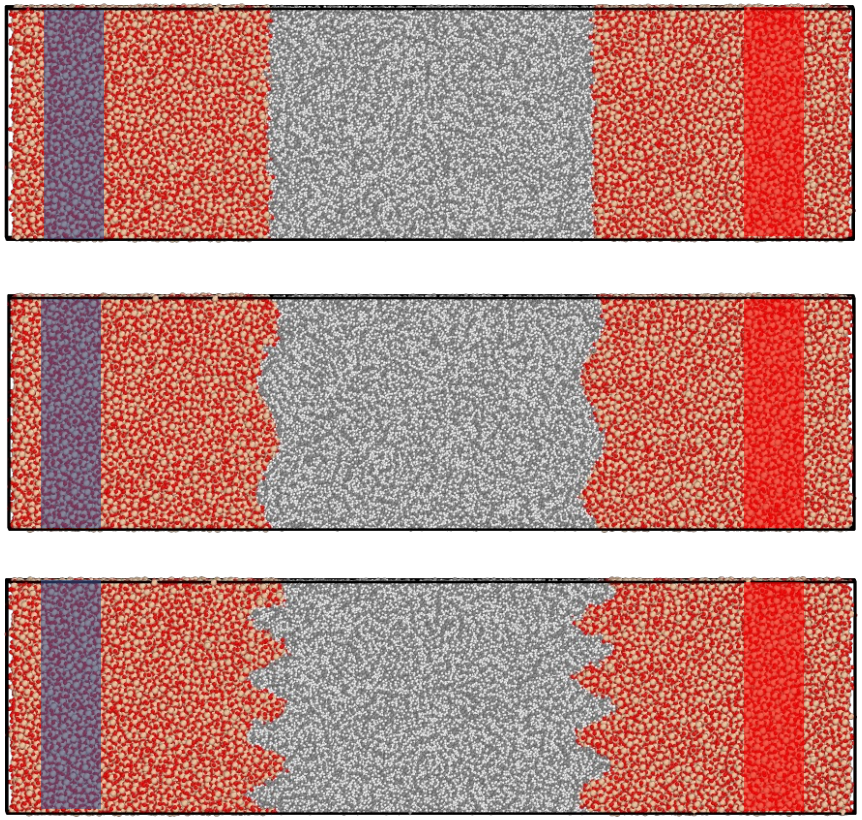


Thermal transport across a nanostructured interface

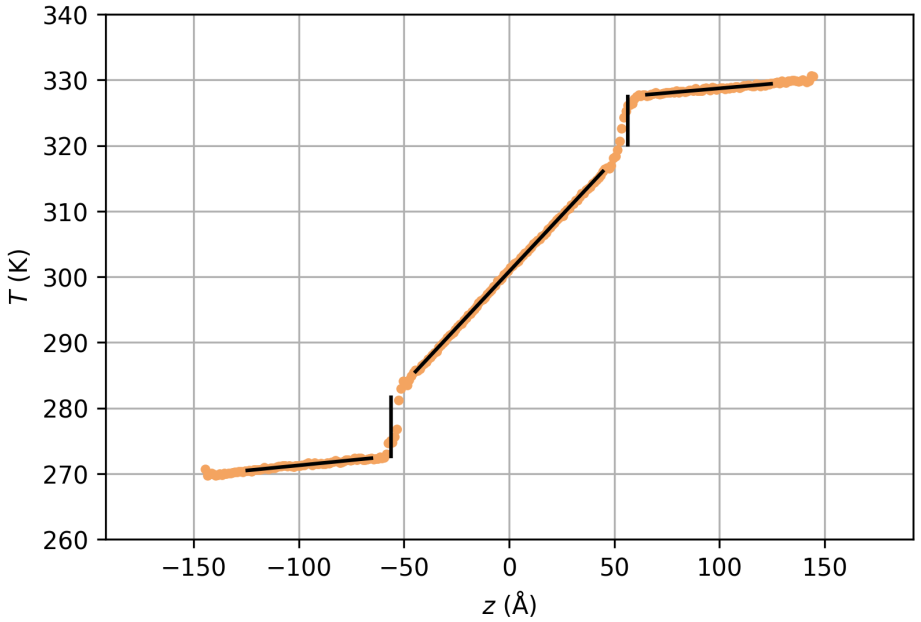
Thermal transport across amorphous silica (SiO2) / hexadecane interface



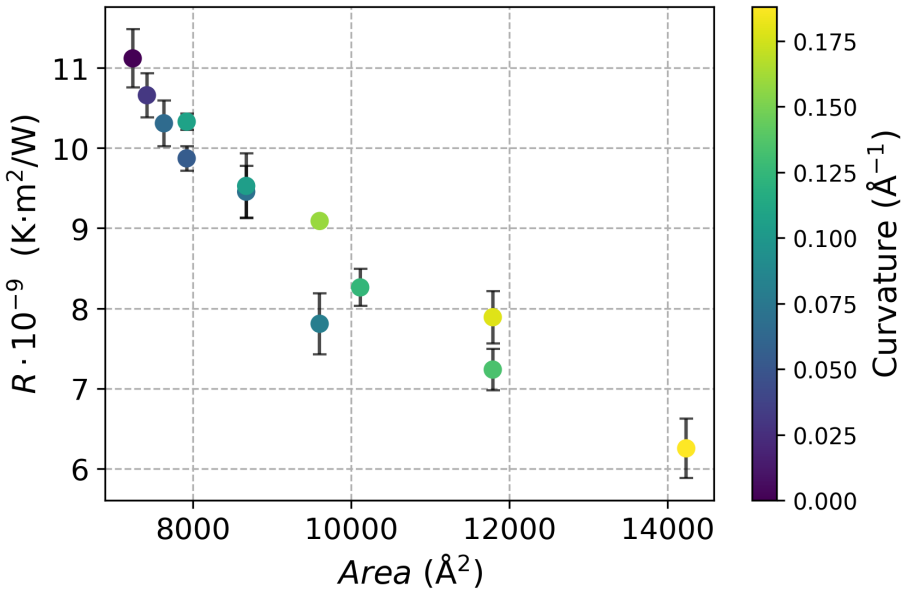
A molecule of hexadecane $CH_3(CH_2)_{14}CH_3$



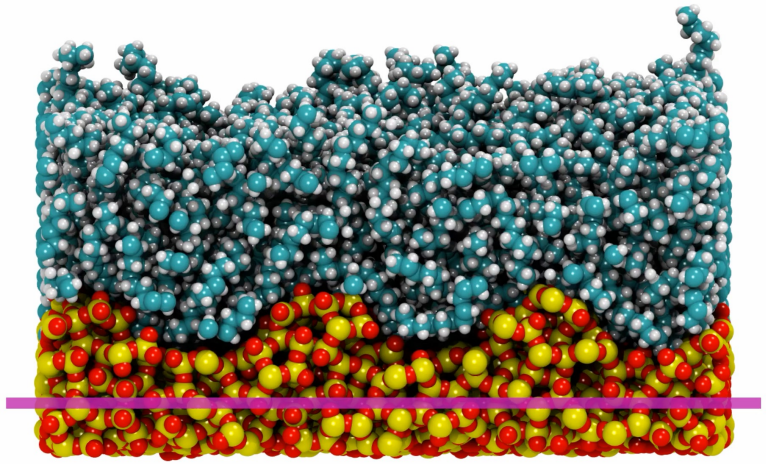
Thermal transport across a nanostructured interface

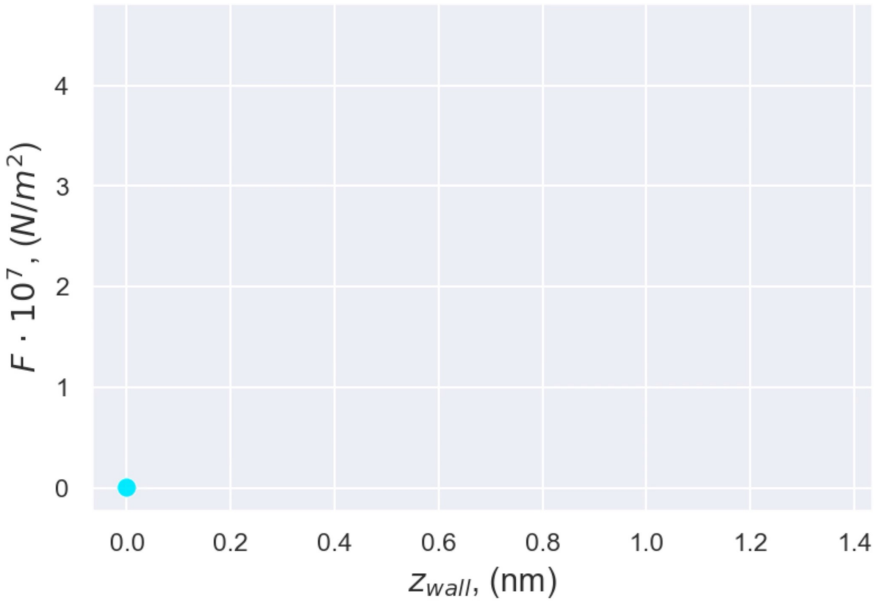


$$R = \frac{\Delta T}{J}$$

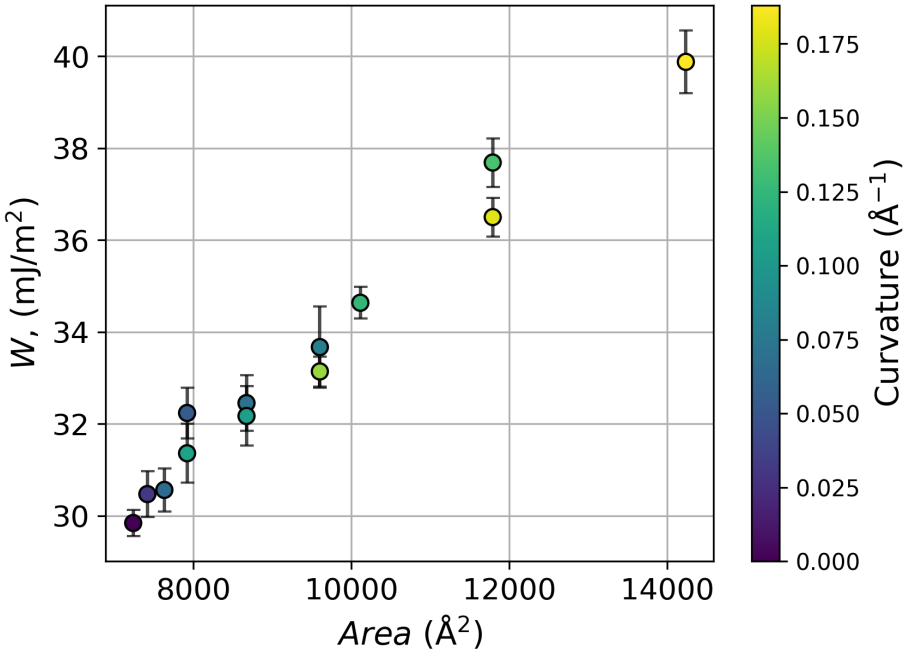


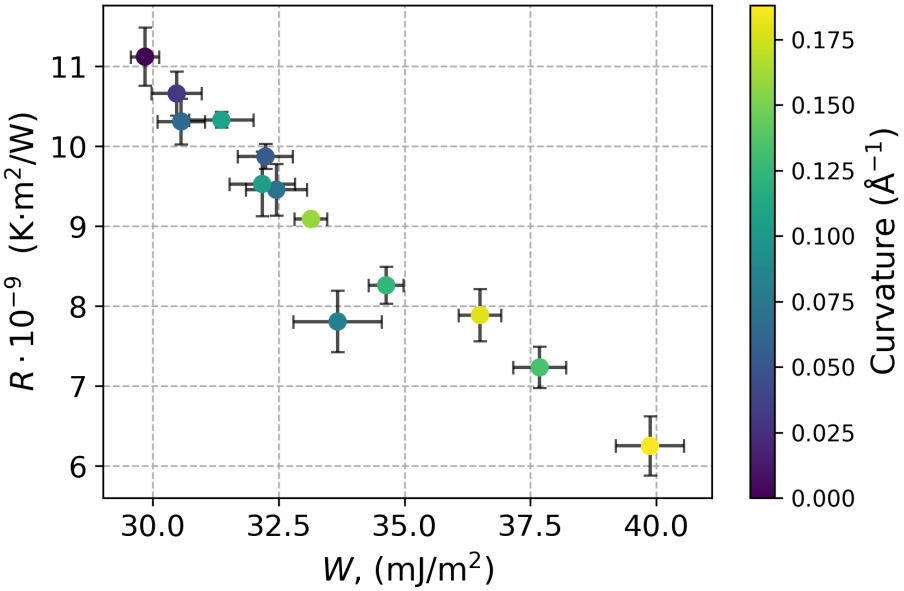
Work of adhesion





Work of adhesion





Conclusions

- We performed molecular dynamics simulations to investigate thermal transport across chemically functionalized and nanostructured solid–liquid interfaces.
- Functionalization of the silica surface with hydroxyl and methyl groups enabled control of the wetting angle over a wide range—from 0° to 130°. This, in turn, led to a variation in the interfacial thermal boundary resistance from approximately 0.5 to 7 × 10^{-9} K·m²/W.
- For nanostructured interfaces, we observed that the interfacial resistance decreases with increasing surface area. Furthermore, a clear dependence of this resistance on the average surface curvature was identified.