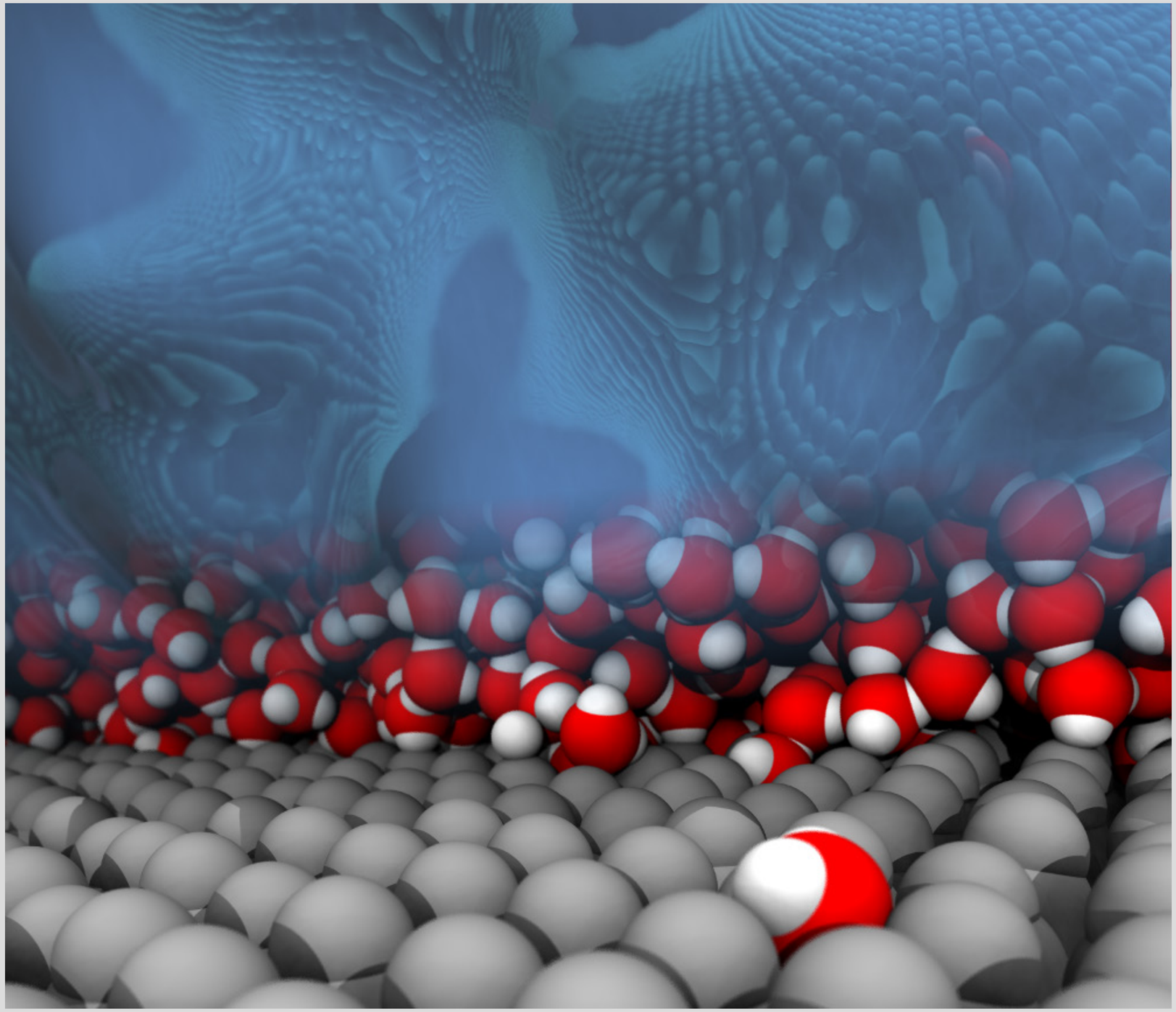
CHARACTERIZING THE DRIVING FORCE OF WETTING

Petter Johansson • Berk Hess

KTH Royal Institute of Technology

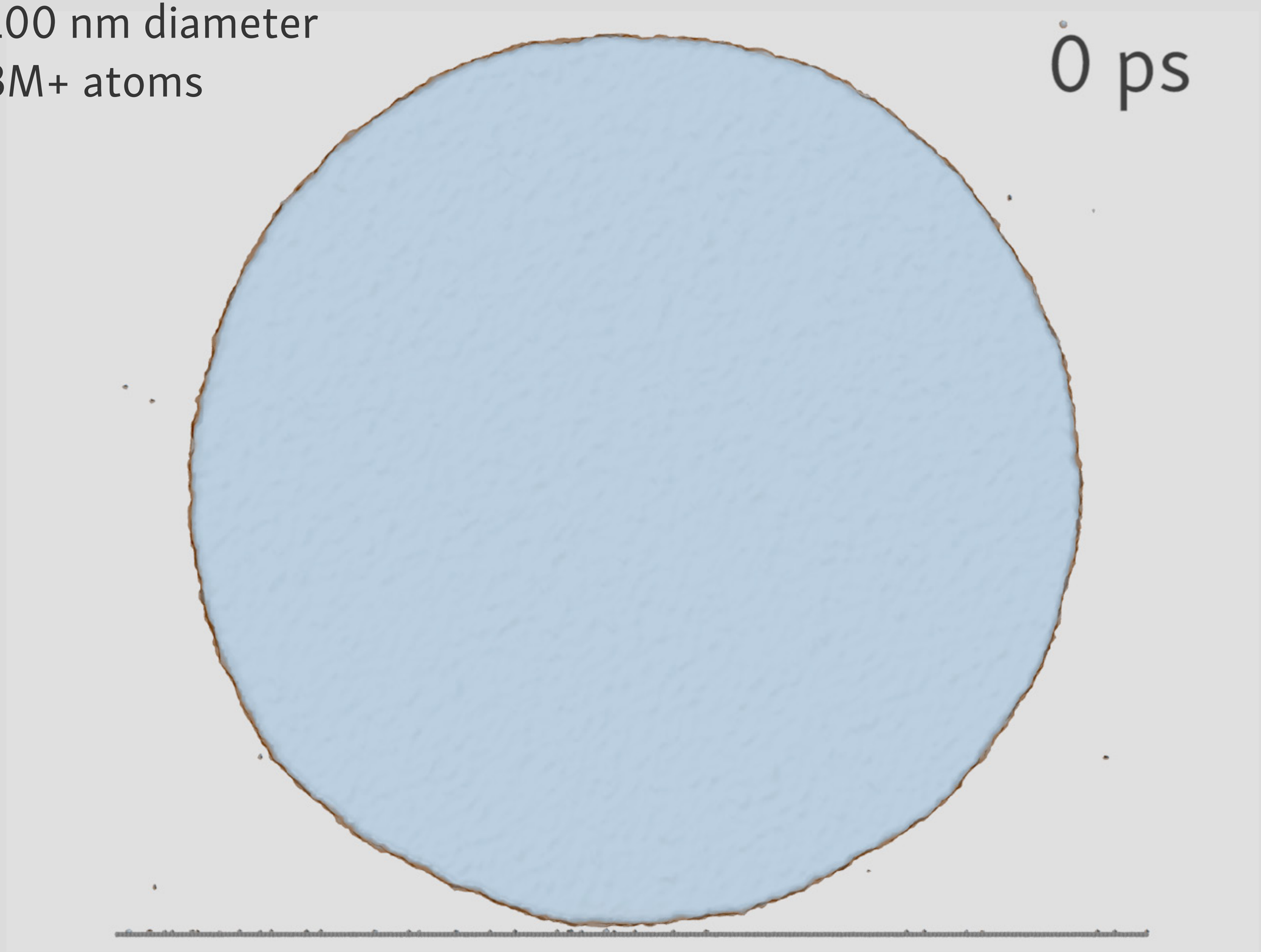
MOLECULAR WETTING

Contact line processes dominate wetting



LARGE SCALE MOLECULAR DYNAMICS

100 nm diameter
3M+ atoms



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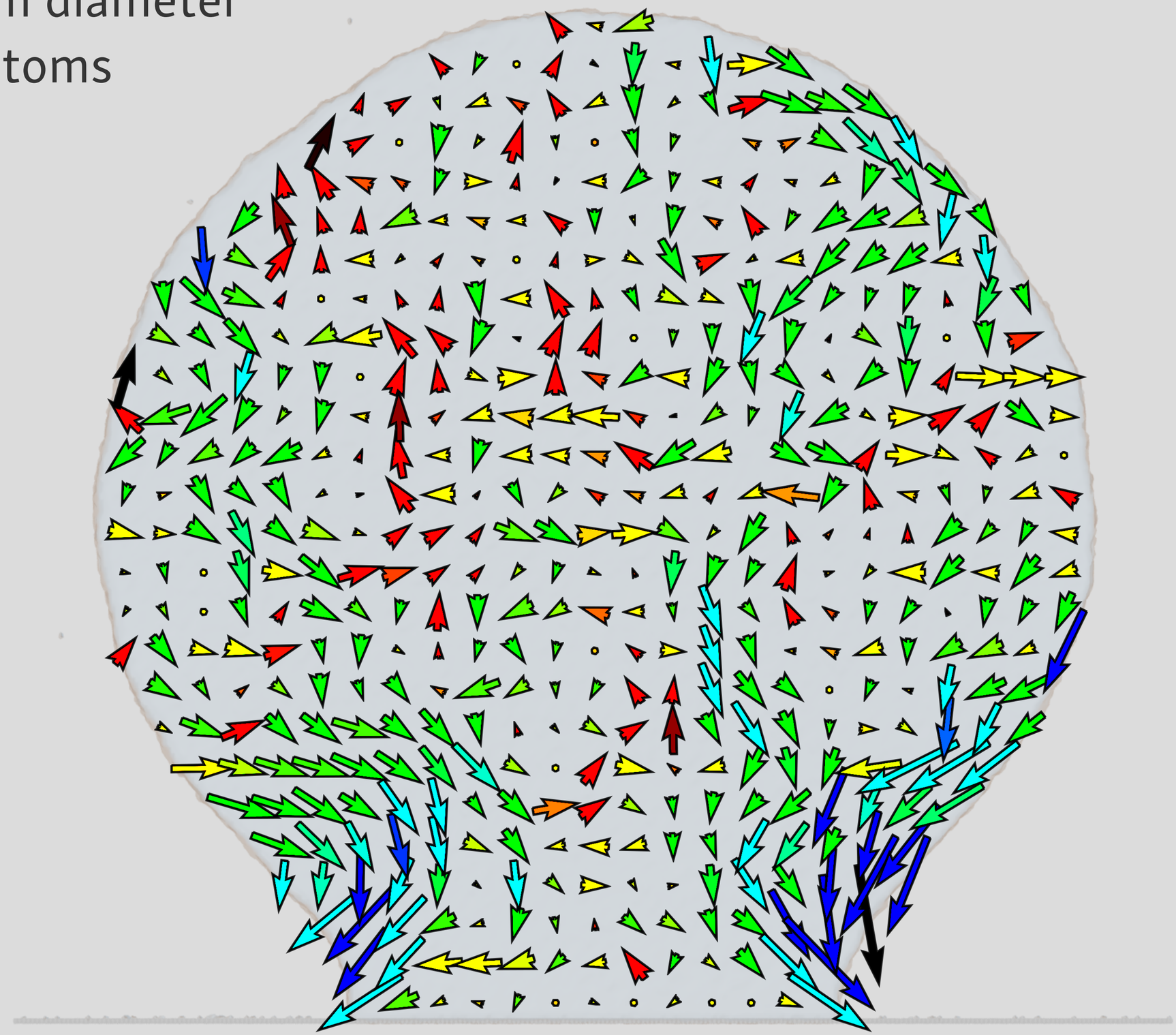
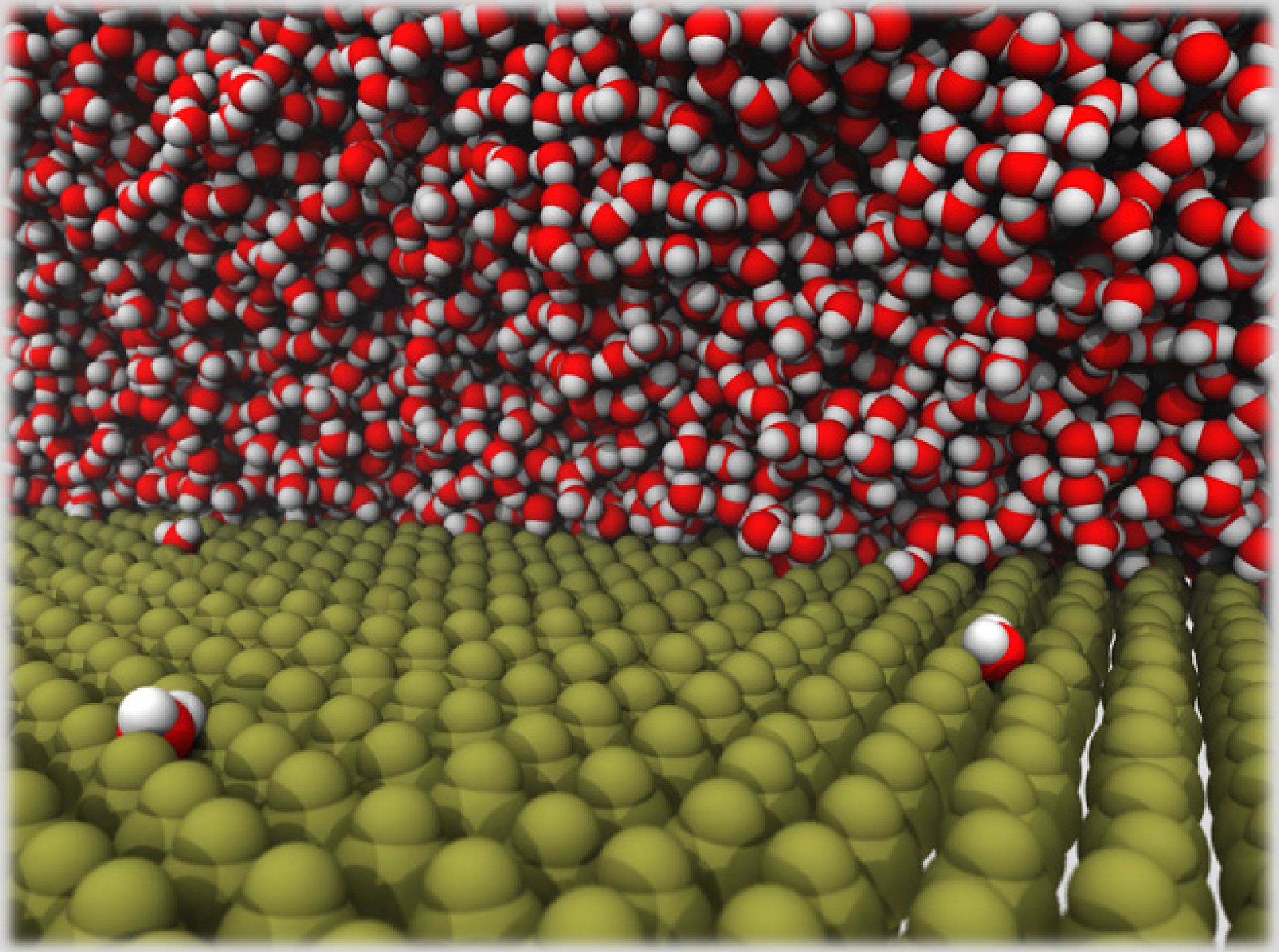
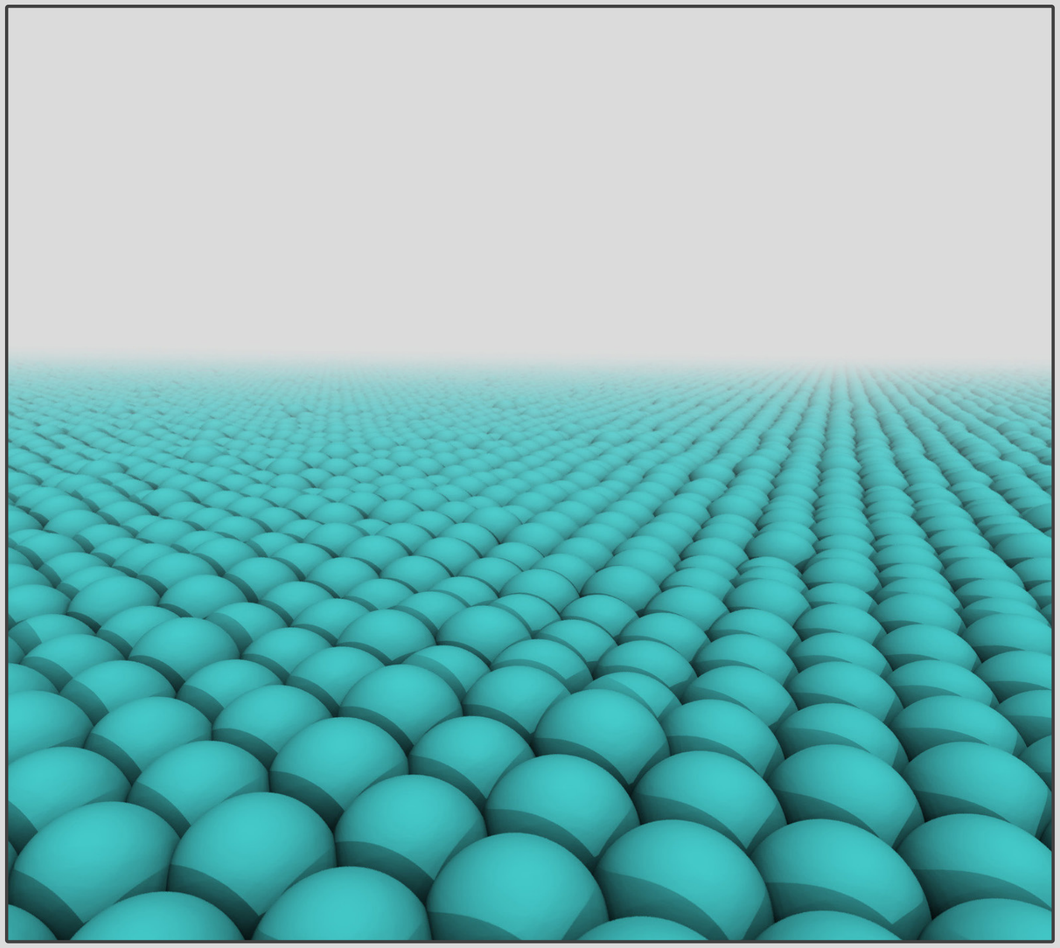


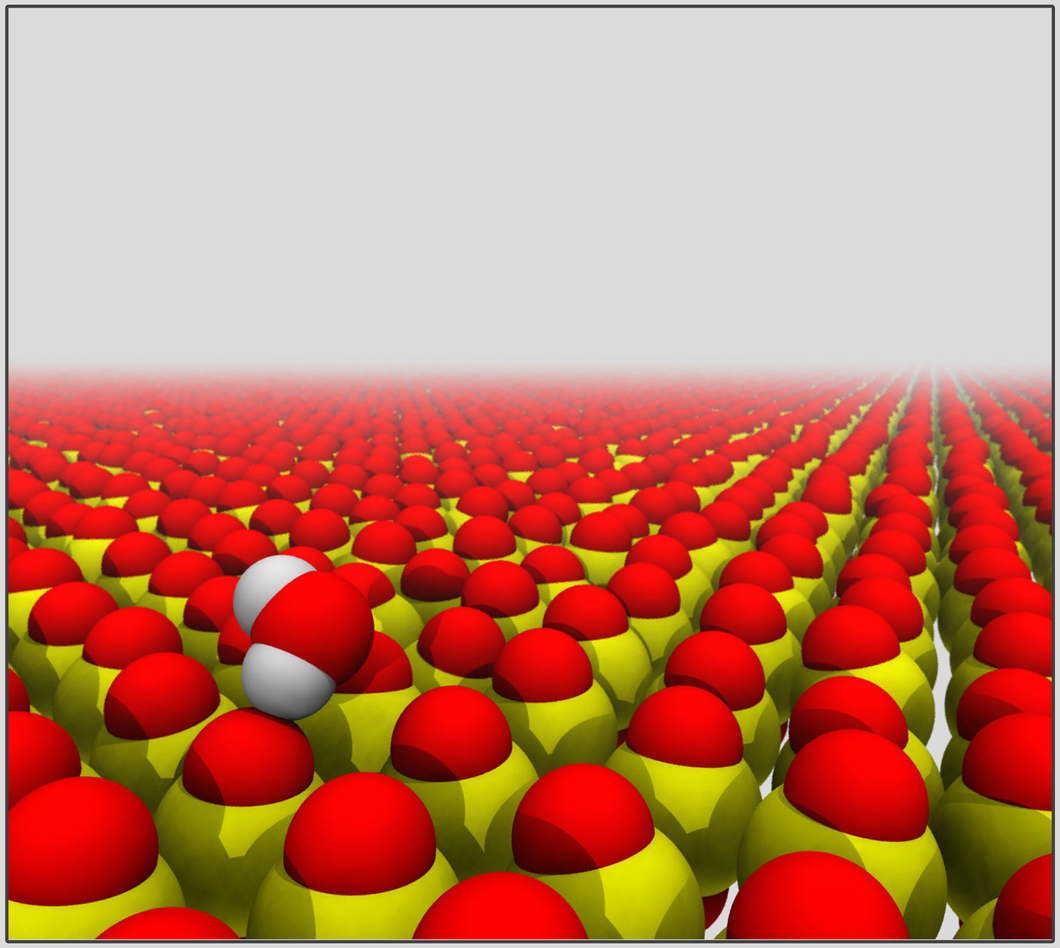


TWO SUBSTRATES



Lennard-Jones atoms

No charges

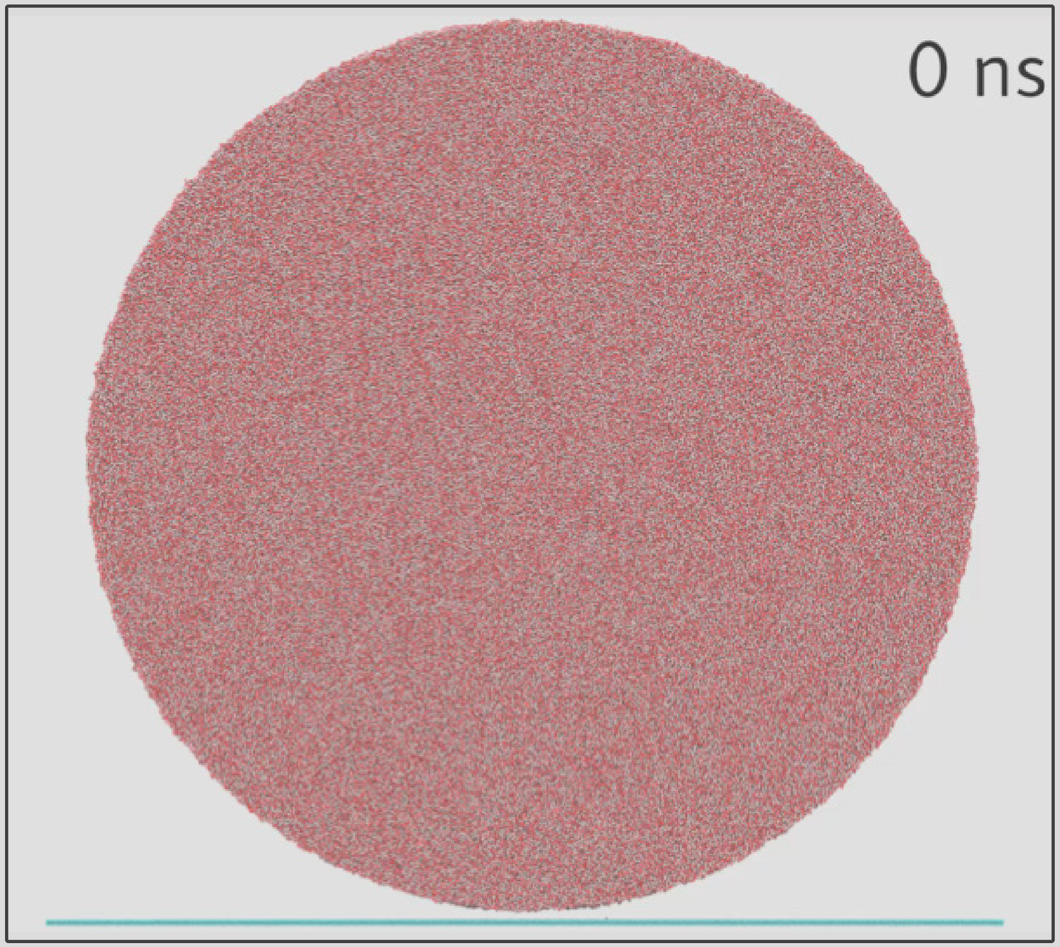


Silica-like (SiO_2)

Charges

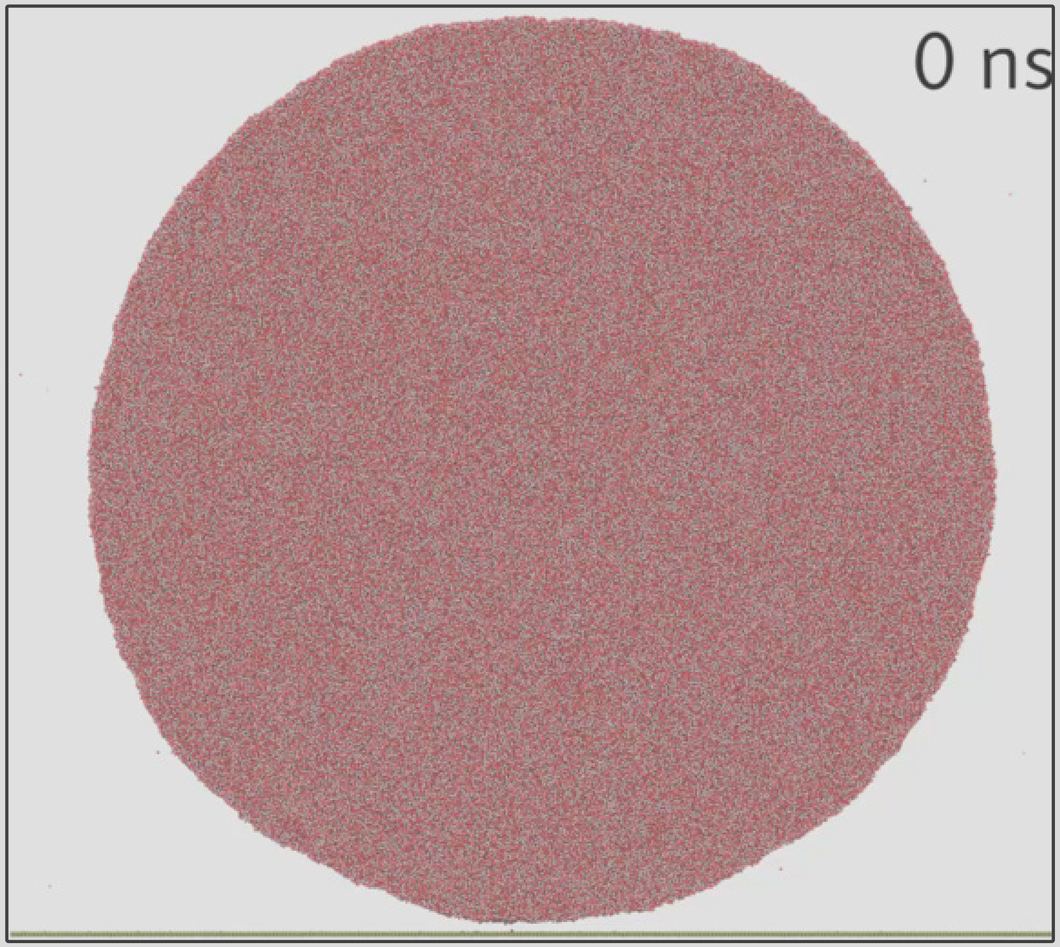
Identical substrate–water interaction strengths (37°)

DIFFERENT RATES



Lennard-Jones atoms

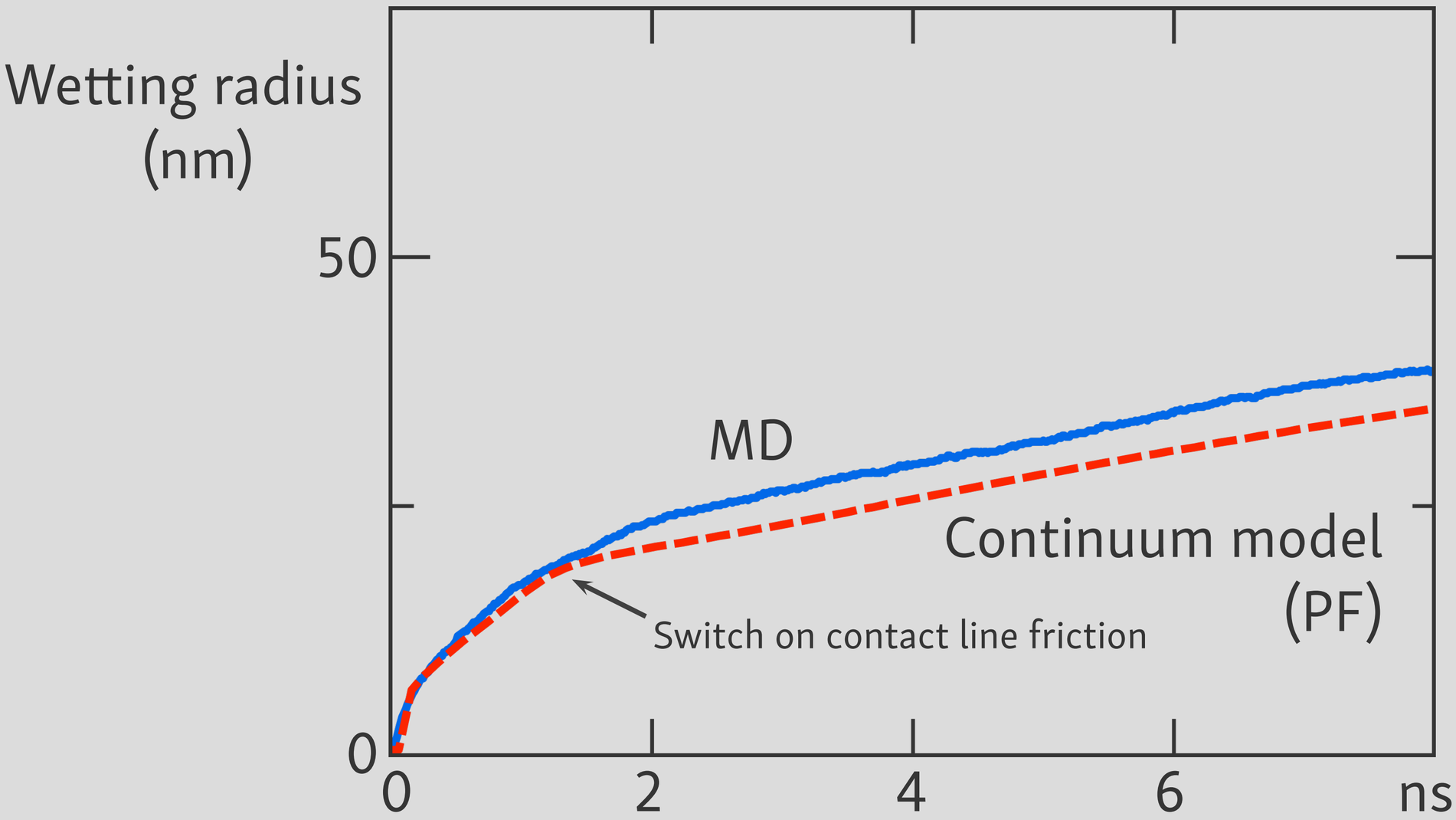
No charges



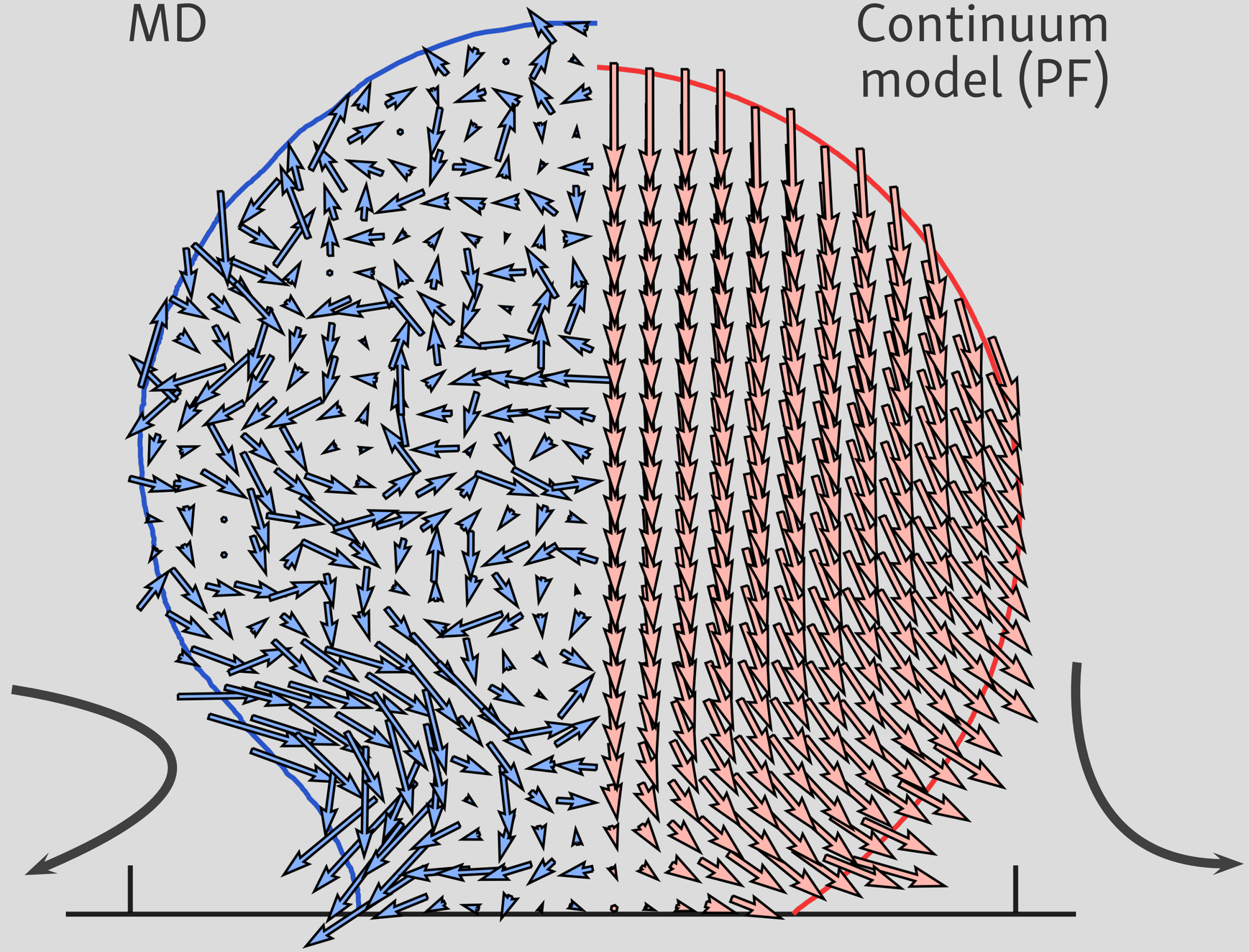
Silica-like (SiO_2)

Charges

Identical substrate–water interaction strengths (37°)



PF model can match rates

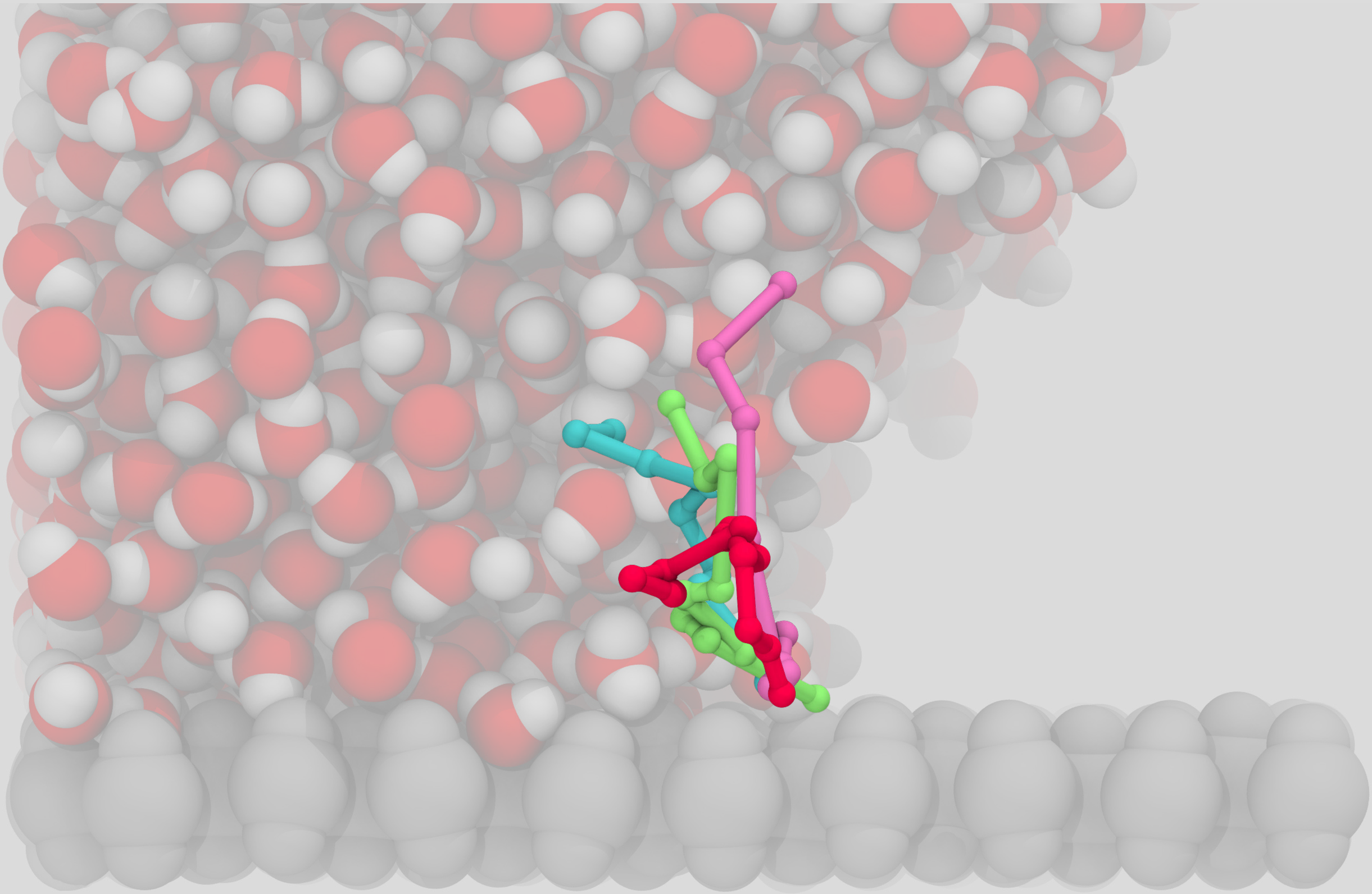


PF model can match rates — *but not dynamics.*

FIRST EFFECT

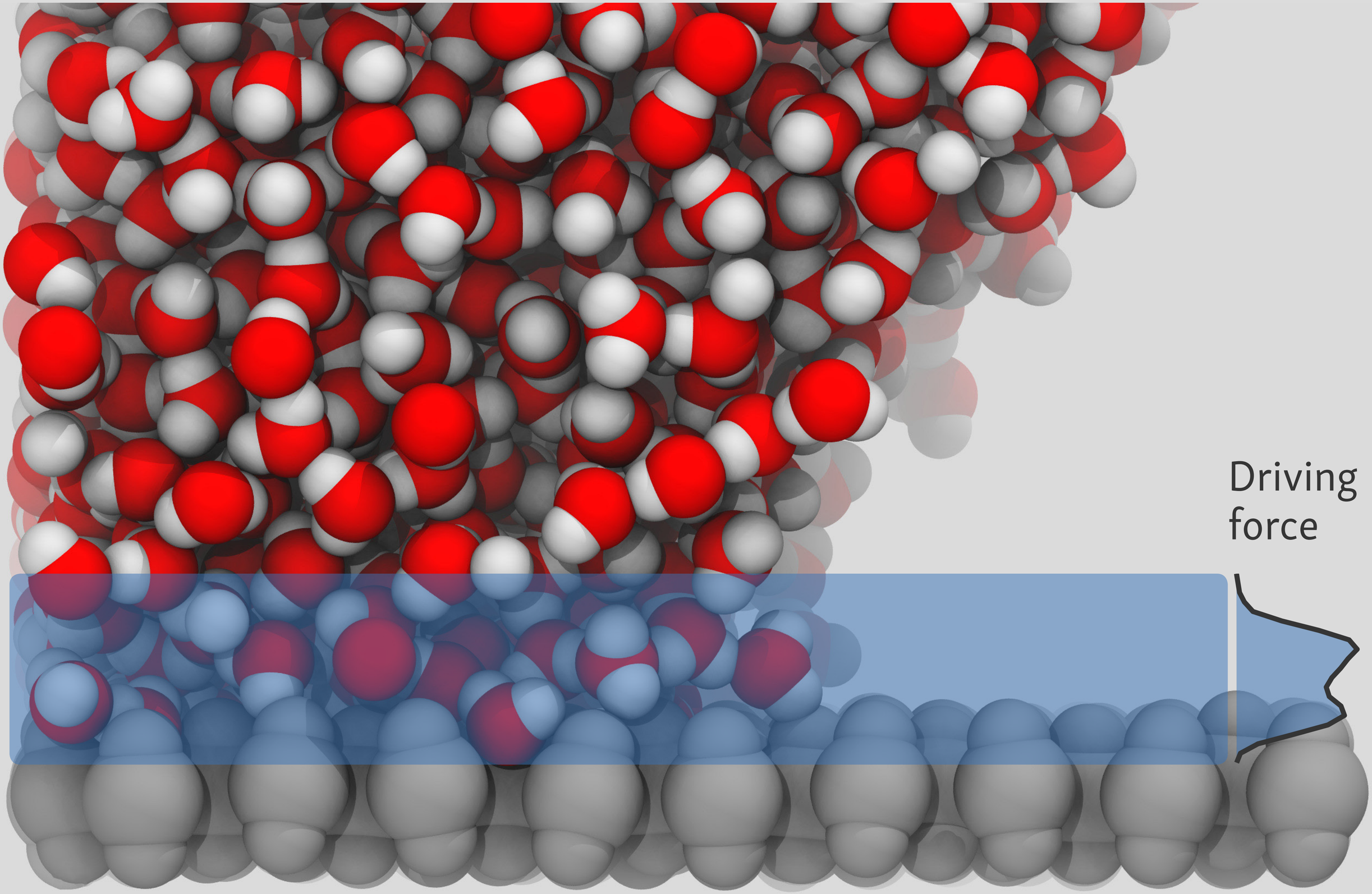
NO-SLIP CONDITION

NO SLIP OBSERVED



SECOND EFFECT

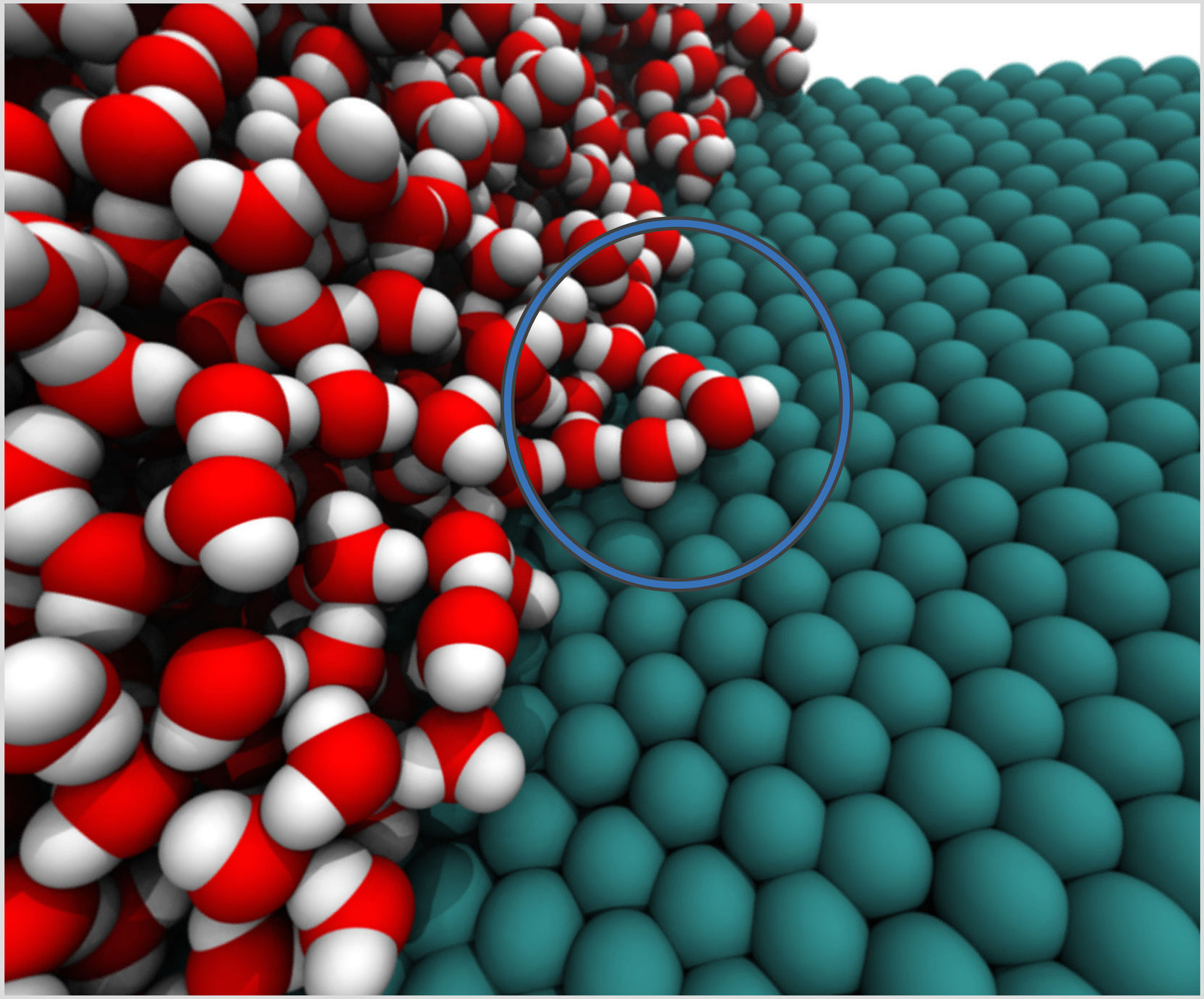
MOLECULAR DRIVING FORCE


Driving
force

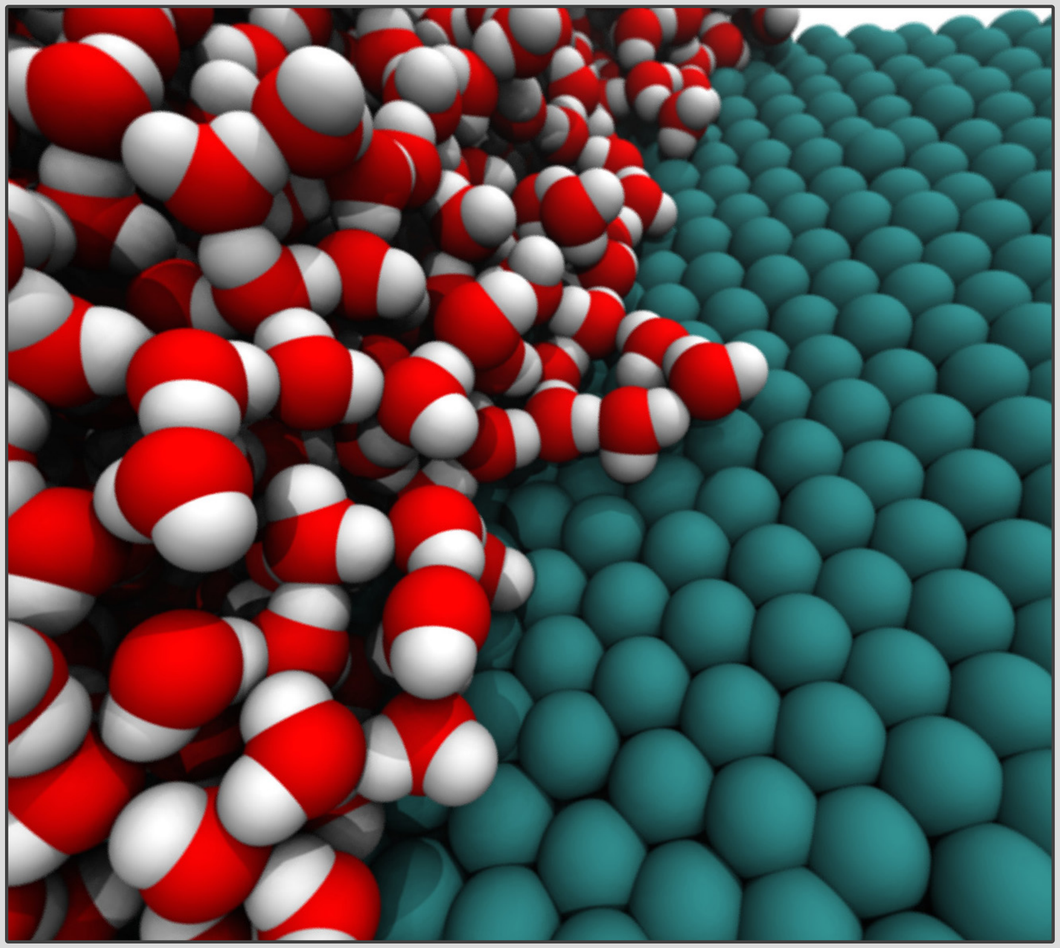
THIRD EFFECT

THERMAL FLUCTUATIONS

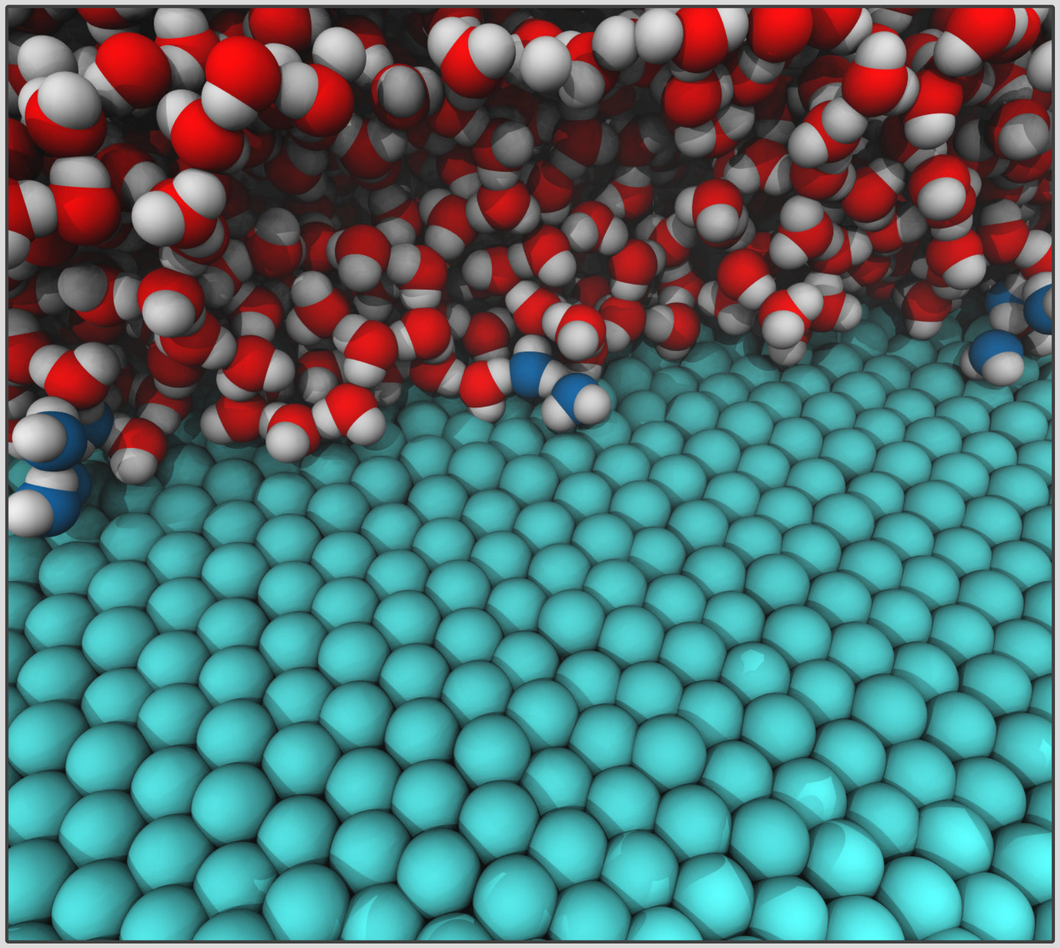
THERMAL NUCLEATION



ENHANCED FLUCTUATIONS



Correct treatment



Artificially amplified fluctuations
2x faster wetting

MOLECULAR EFFECTS

- No-slip condition holds on silica-like.
- Driving force is very short ranged.
- Thermal fluctuations an important effect.
- PF model not matching MD dynamics.

P Johansson, A Carlson, B Hess (2015). Journal of Fluid Mechanics, 781, 695–711.

ACKNOWLEDGEMENTS

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KTH VETENSKAP OCH KONST

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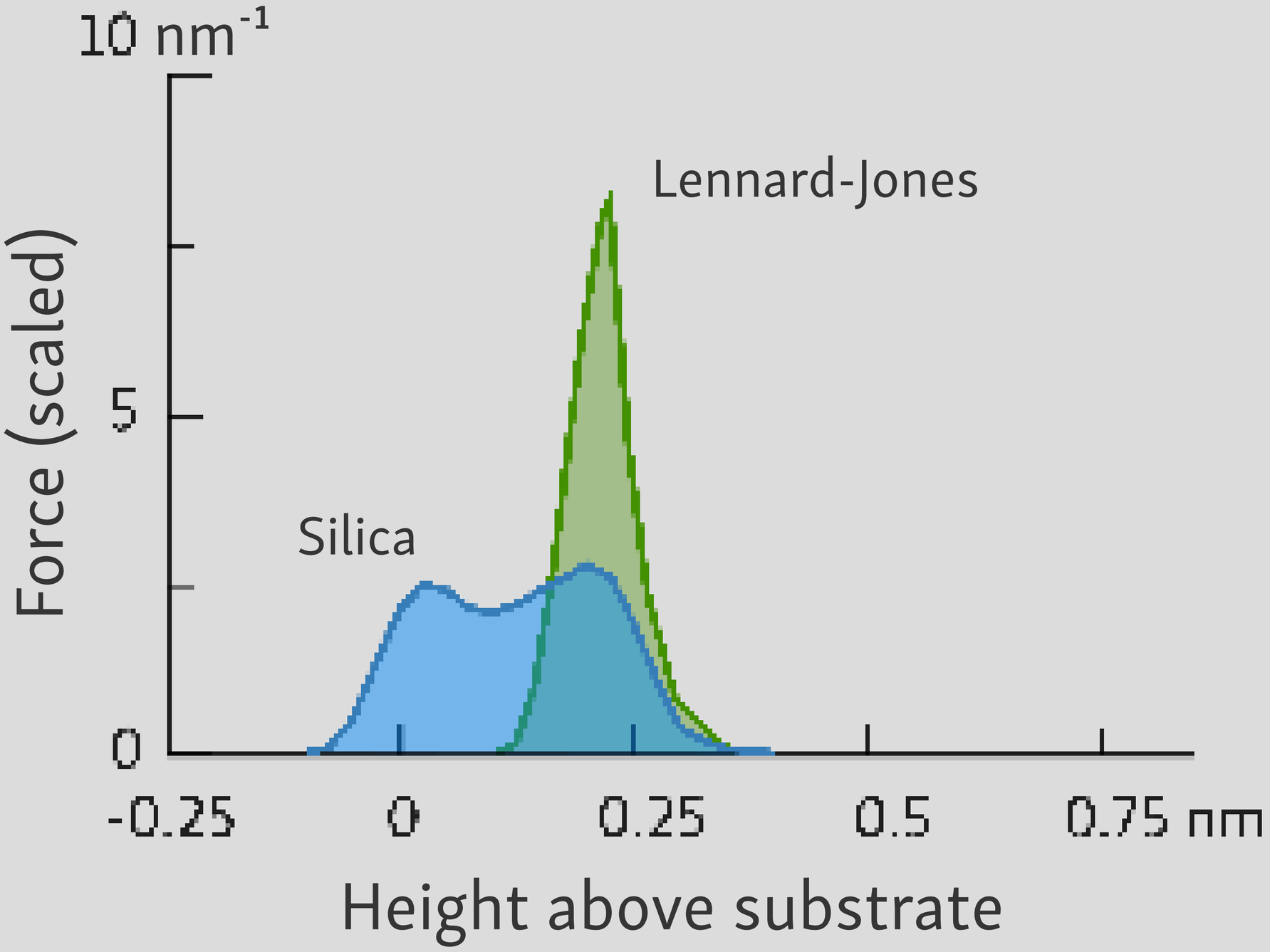
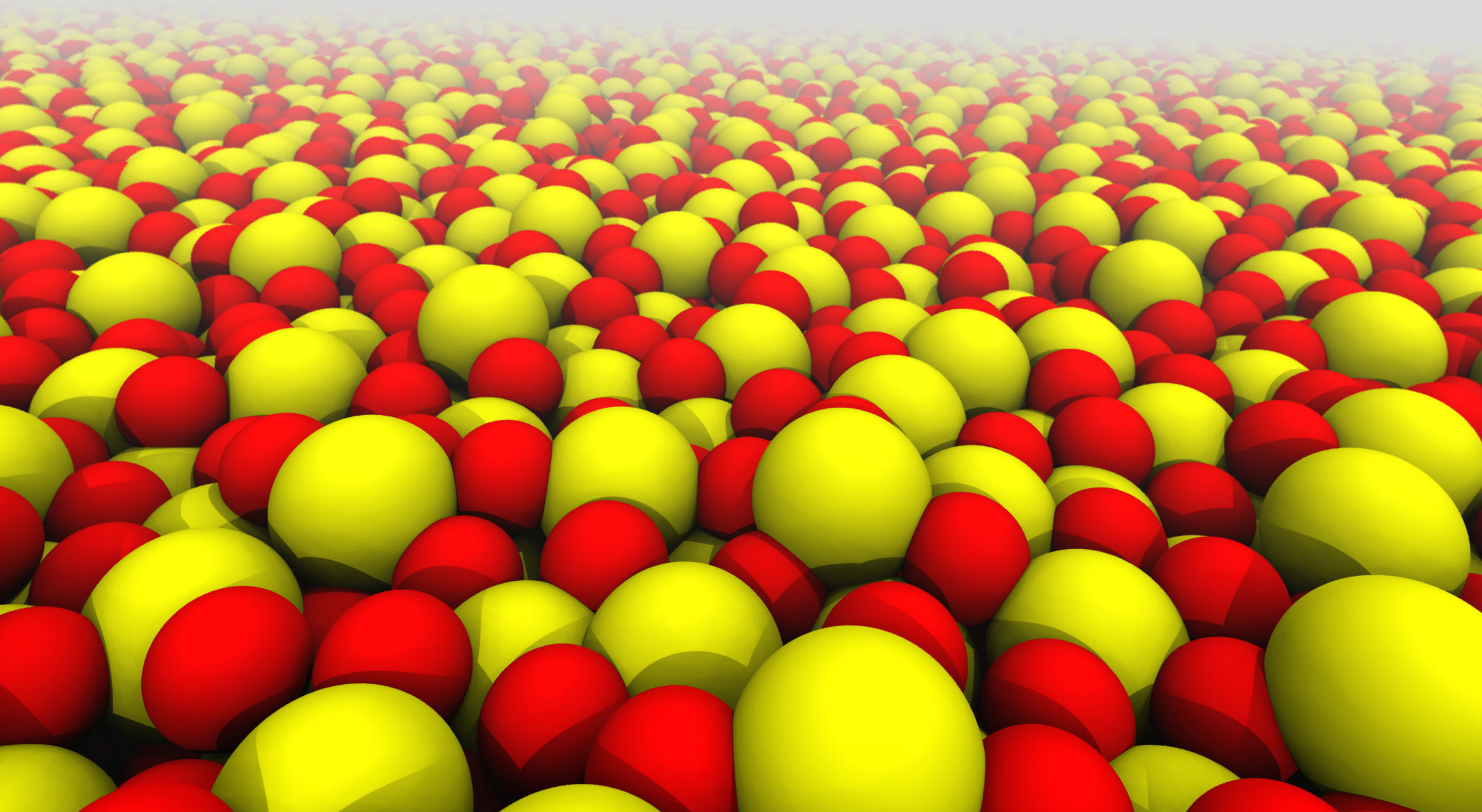
THANK YOU!

MEASURED FORCE



A “REALISTIC” SILICA



MOLECULAR DYNAMICS