Molecular Dynamics Driven Screening of Wettability for Passive Cooling

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1 Introduction

Project Context

Electricity use for space-conditioning is expected to triple by 2050[1]

Near-Zero-Carbon, All-Climate-Adaptive Air-Conditioning (NZC-AC-AC) Project with the University of Bath and the University of Hull.

- **Goal:** Replace vapour-compression with capillary-driven evaporative cooling
- **Impact:** 80-90 % energy bill savings, near-zero carbon emissions
- **Scope: Molecular Dynamics (MD)** Screening stage of Phase 1

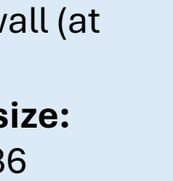
NZC-AC-AC **Phase 1 of 5**

Candidate Materials → **MD-screening & Simulation** → Refinement → Composition & Combination Methods Development; Characterisation & Selection

Experimental contact-angle (θ) tests are slow and error-prone (surface heterogeneity, operator bias)[2]

Need: Fast method to assess wettability of materials

Solution: Fast, Reproducible MD-Based Screening



2 Aims & Objectives

- Develop a foundation for a reusable, high-throughput MD framework for rapid contact-angle prediction
- Validate a water model with VLE to be used in the MD pipeline
- Assess how surface-atom density, wall chemistry, temperature, and droplet size jointly influence wettability on **implicit** walls.
- Validate MD-predicted qualitative trends against established trends and experimental data.
- Setup diffusion and explicit wall simulations for future work

3 Methods

Simulation Workflow

GROMACS 2018.2

Create Simulation Box → Set desired input parameters → Energy minimisation step → **VLE Analysis** / **Contact Angles**

VLE Analysis: Run NVT simulation with SPC model → Extract density data using **XMGrace**

Contact Angles: Run NVT simulation with TIP4P model → Visualise output file in **VMD** → Measure contact angles

- NVT ensemble
- Berendsen Thermostat
- Timestep: 2 fs (200 ps total)
- Implicit Walls: 9-3 Potential

VLE simulations: 278 – 517 K

Contact Angle Simulations:

- **Temperature:** 50 – 200 atoms nm^{-3} at 278, 298, and 318 K (Carbon wall)
- **Atom Type:** 50 – 200 atoms nm^{-3} with PFAS and Oxygen wall (at 298 K)
- **Droplet size:** 216 – 5186 molecules at 298 K (Carbon wall).

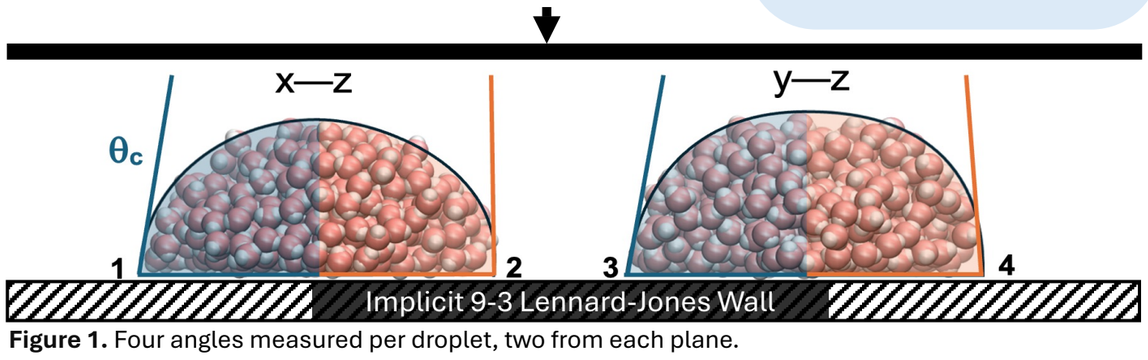


Figure 1. Four angles measured per droplet, two from each plane.

4 Results

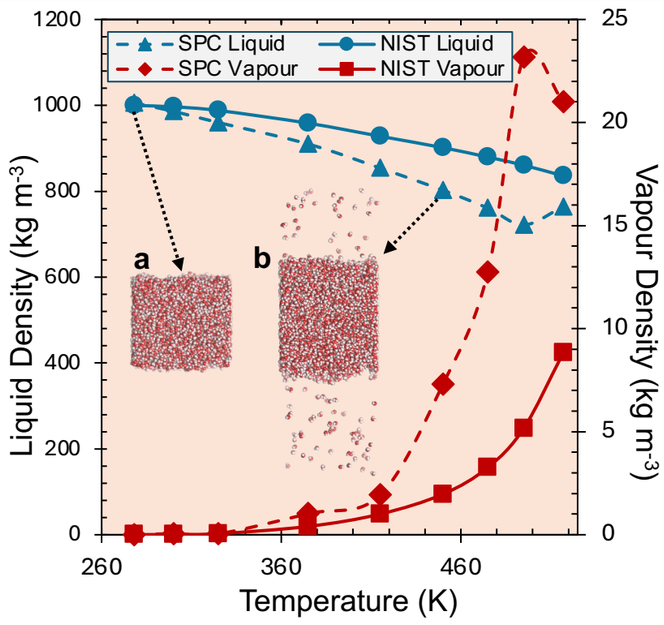


Figure 2. VLE curves 278-517 K for SPC water model compared against NIST data. Inset a) SPC at 278 K, Inset b) SPC at 450 K.

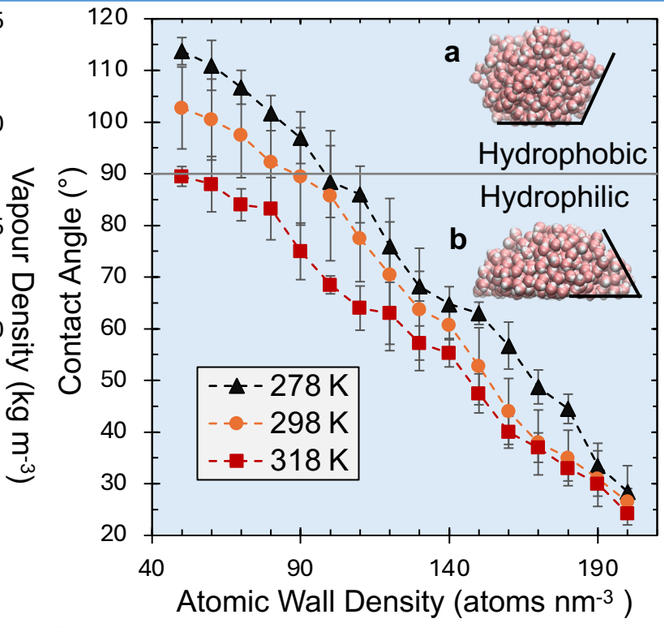


Figure 3. Contact angle θ vs. atomic wall density at 278 K (▲), 298 K (●), and 318 K (■). **a)** Hydrophobic droplet **b)** Hydrophilic droplet

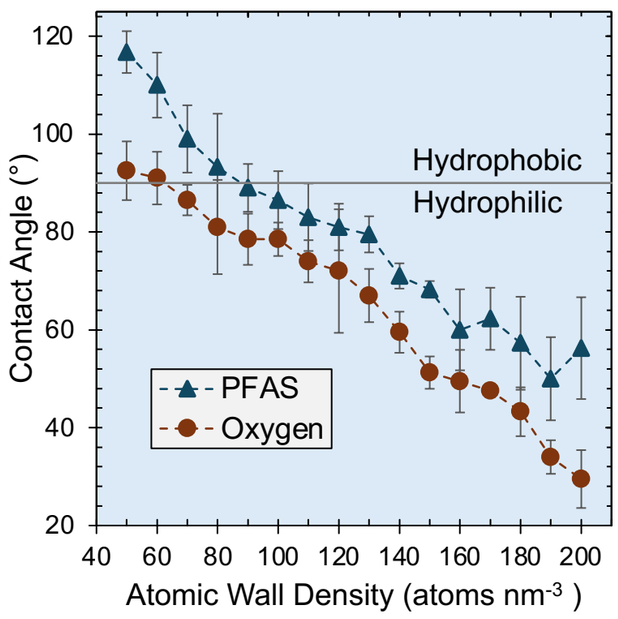


Figure 4. Contact angle θ vs. atomic wall density for PFAS (▲), Oxygen (●) like surfaces.

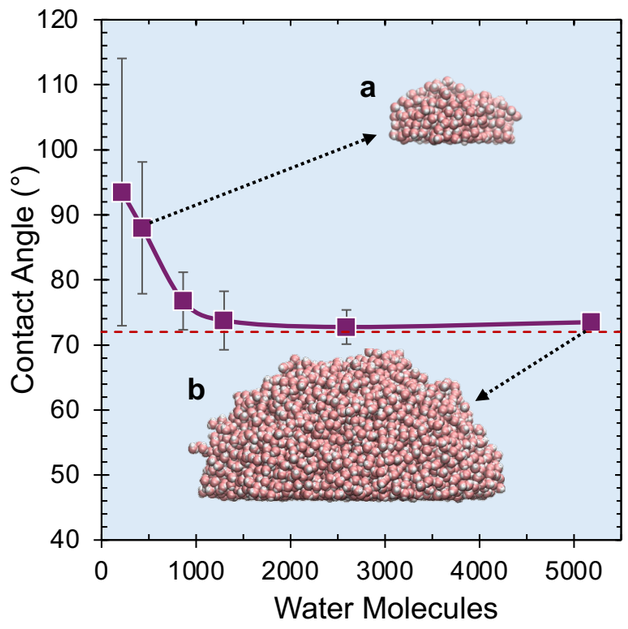


Figure 5. Contact angle θ vs. droplet size (216 – 5186 molecules). **a)** 416 molecules, **b)** 5186 molecules

5 Conclusions

- **TIP4P water model** with implicit walls reproduce ρ_s–θ trends with $R^2 > 0.97$. The qualitative trends align with experimental literature for similar hydrophobic[3] and hydrophilic surfaces[4].
- **Structural lever** (ρ_s): $\Delta\theta/\Delta\rho_s$ = 0.45–0.58° per atom·nm^{-3} (0.45° at 278 K, rising to 0.58° at 318 K), indicating greater sensitivity at lower temperatures.
- **Chemistry effect:** At identical densities, PFAS-like C remains ~14° ± 5.2° more hydrophobic than O walls
- **Size scaling:** Above ~6 nm droplets (2 000 H_2O), Δθ with size is < ± 3°. Convergence wasn't expected at such few molecules
- Initial **diffusion** and **explicit** wall simulation boxes were setup to help guide the future work.
- Importantly, we show that this MD framework can guide early material selection with fast simulations before employing more computation on explicit wall simulations.

Quantitative θ should be validated with explicit-wall MD or experiment; the trends in this study are robust for triage purposes.

6 Future Work

- Conduct humid-air simulations (Figure 6) to calculate multicomponent diffusion coefficients.
- Incorporate explicit atomistic walls (Figure 7) with mixed chemistries to validate and obtain quantitative predictions
- Couple atomistic insights with pore-scale performance metrics to guide sustainable cooling bed design.

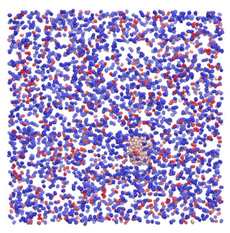


Figure 6. 63% RH, 293 K, 1 bar 18x18x18 nm simulation box with water oxygen and nitrogen.

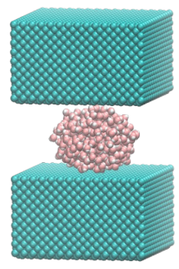


Figure 7. 5 x 5 x 5 nm simulation box of water in a pore with explicit carbon walls.

Acknowledgements

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References

1. IEA, The Future of Cooling. (2018).
2. T. Huhtamäki et al., Nat. Protoc. 13, 1521 (2018).
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4. B. L. Zhuravlev, Colloids Surf. A 173, 1 (2000).

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