Hydrophobic Forces on the Molecular Scale I

Dominik Horinek, Andreas Serr, Roland Netz
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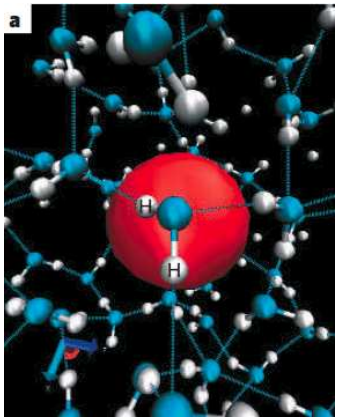
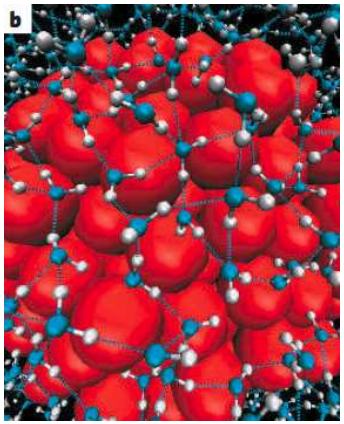
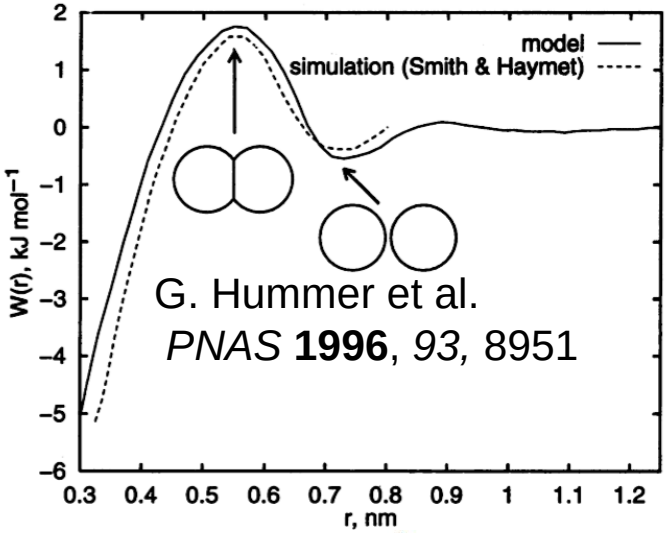
Small cavities



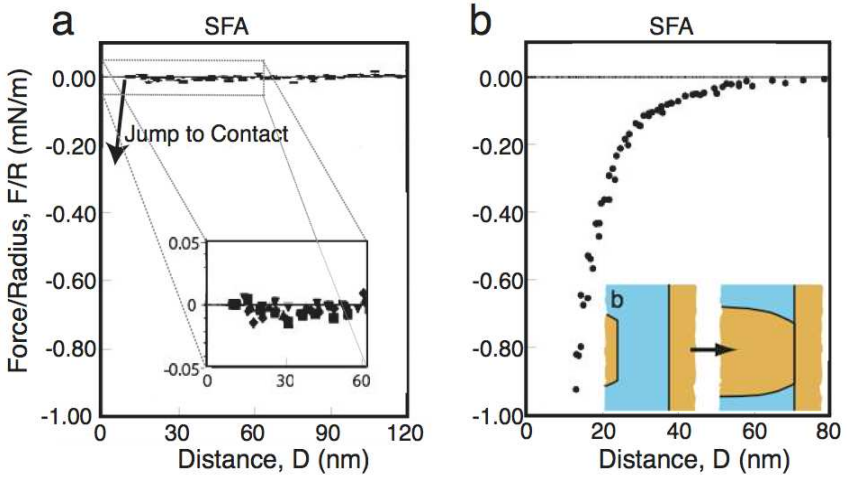
Large cavities



D. Chandler, *Nature* **2005**, *437*, 04162



G. Hummer et al.
PNAS **1996**, *93,* 8951



E. E. Meyer, K. J. Rosenberg, J. Israelachvili
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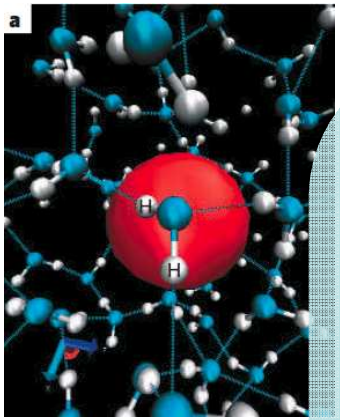

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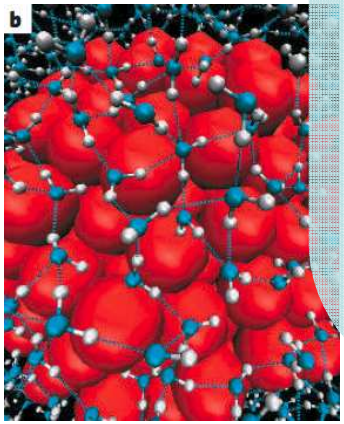

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What does this tell us about the hydrophobic attraction for real ions, molecules, polymers?

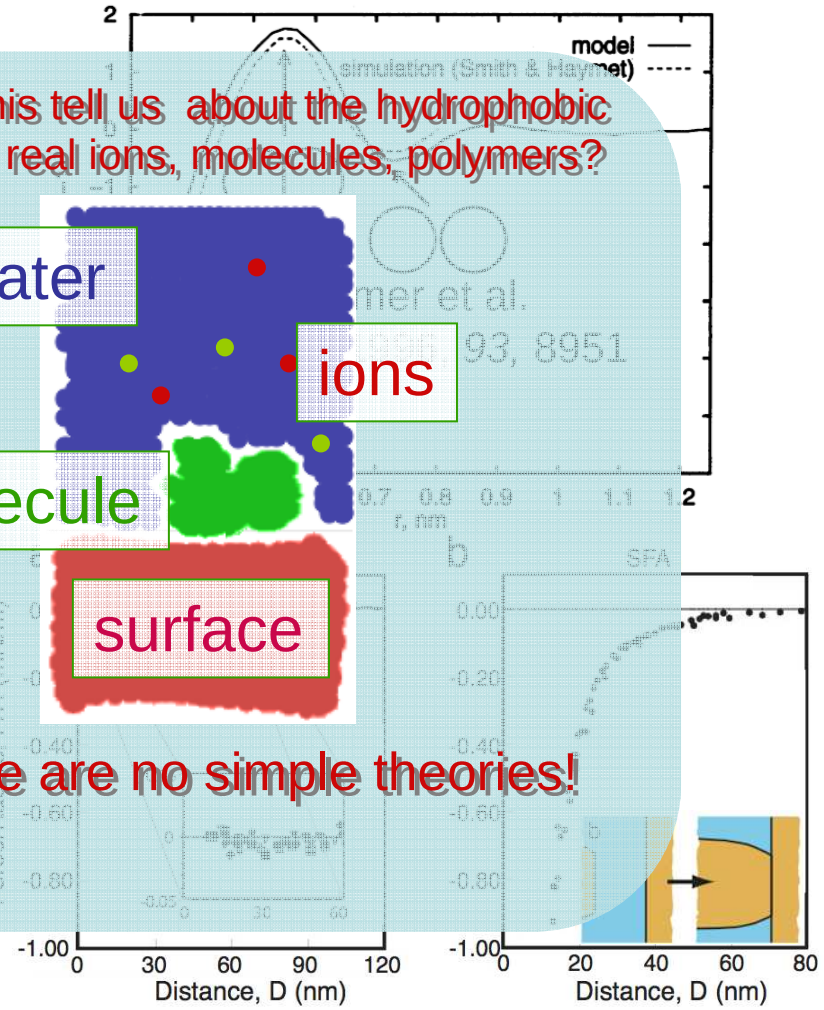
water

ions

molecule

surface

There are no simple theories!



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Hydrophobic Forces on the Molecular Scale II

Ions

6×8 icosane SAM with a 30º tilt angle.

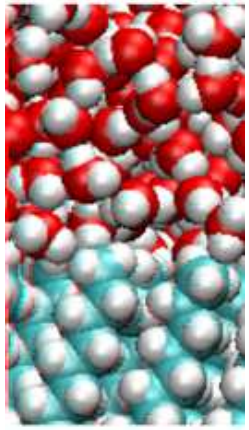
General Amber force field

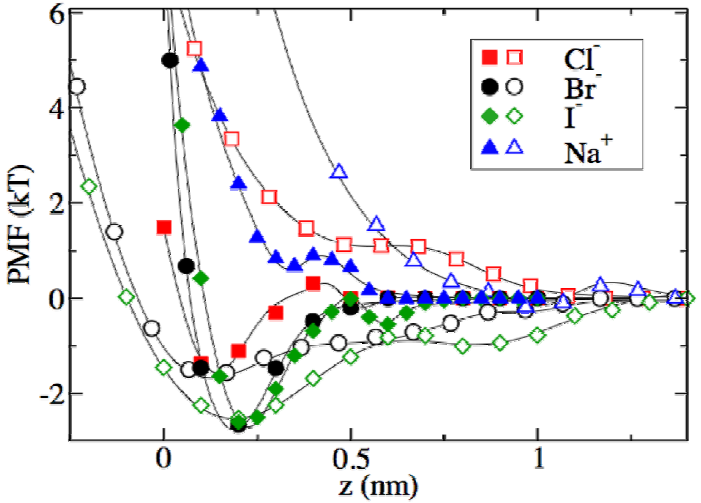
Polarizable POL3 water model

Polarizable Ion parameters

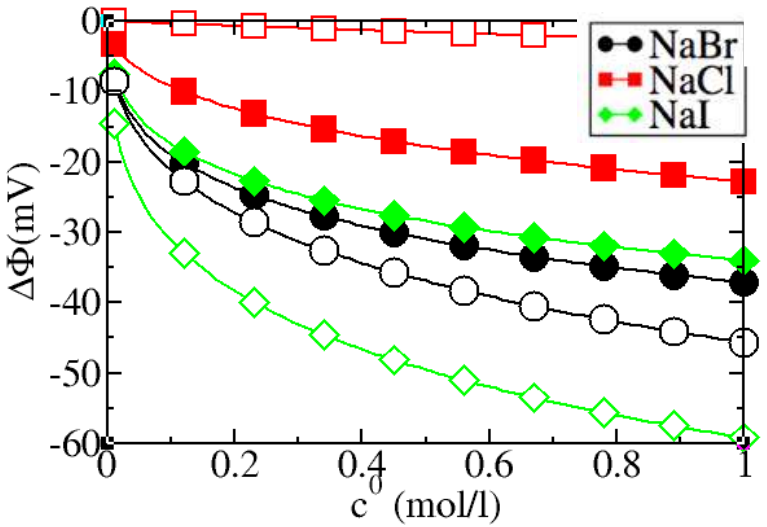
Potentials of mean force for a single ion are calculated by umbrella sampling

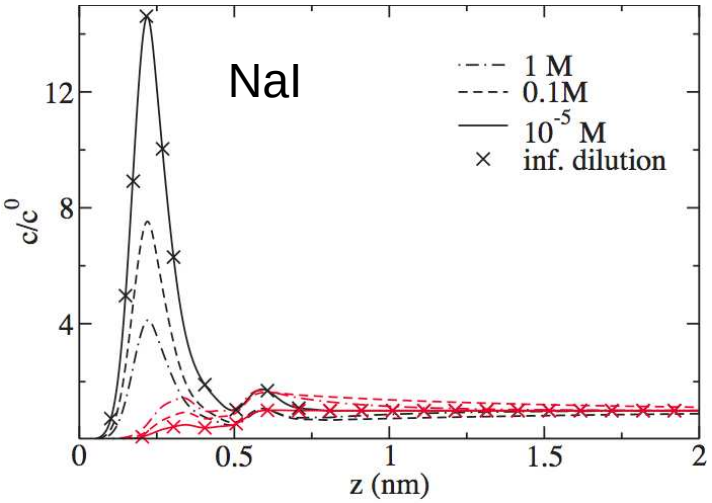
Extended Poisson-Boltzmann modeling for finite salt concentrations





■ SAM □ air (LX Dang)

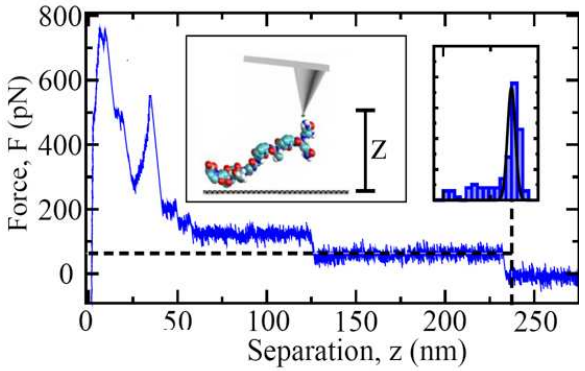




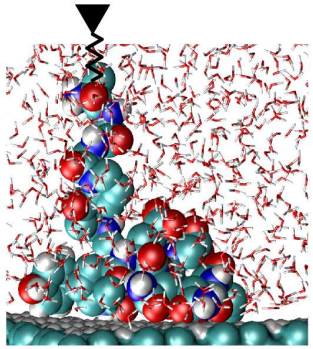
Qualitative agreement with experiments

Hydrophobic Forces on the Molecular Scale III

Peptides



AFM experiment: C_{16} silk protein, diamond surface (T. Hugel, TUM)



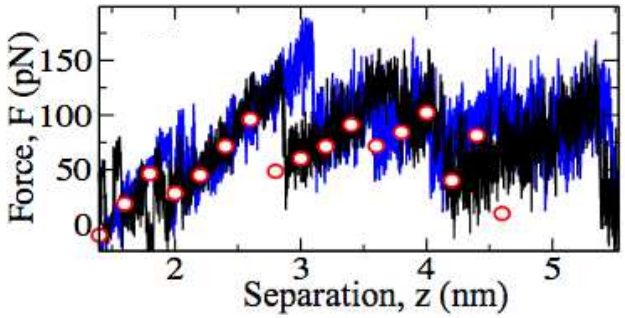
Simulation snapshot

On hydrophobic surfaces, equilibrium forces can be obtained:

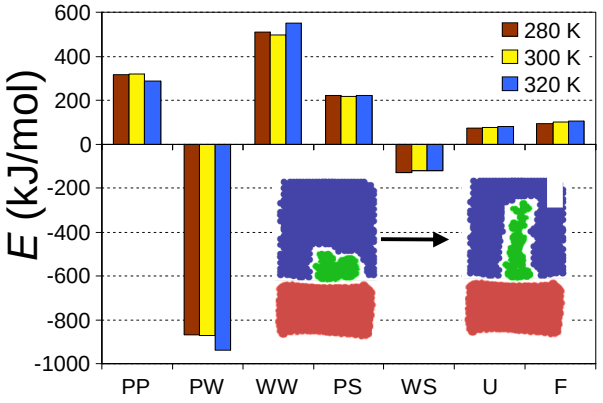
<F> = 58 pN (Exp)

<F> = 54 pN (Sim)

Simulation details: - atomistic resolution
- AFM tip modeled by a harmonic potential
- Gromos96 and SPC force fields



MD force/extension curve



Energy analysis

Conclusions: atomistic MD is able to predict hydrophobic attraction of complex biomolecules