# Ice and Liquid Water at Interfaces

Angelos Michaelides
*Thomas Young Centre,*
*London Centre for Nanotechnology & Department of Chemistry,*
*University College London (UCL), UK*

*main collaborators:*

*Ming Ma, Gabriele Tocci, Laurent Joly (Lyon)*

**www.chem.ucl.ac.uk/ice**

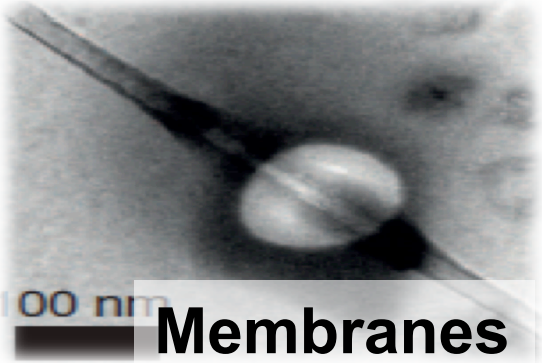
# Water-solid interfaces are ubiquitous

Earth Science


Energy

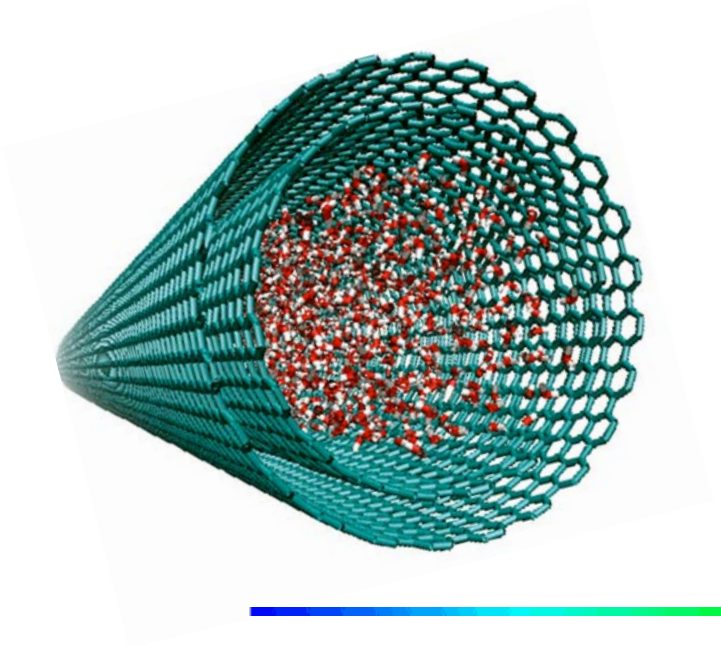
Corrosion

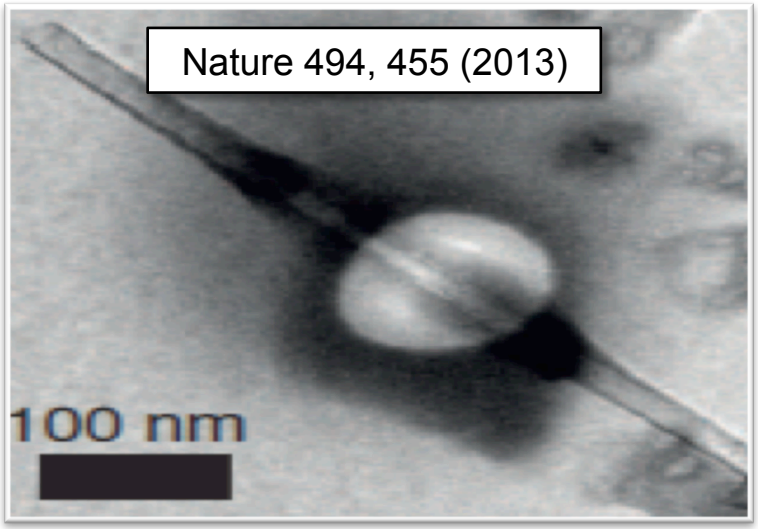
## Major gaps in understanding at the molecular level




Membranes

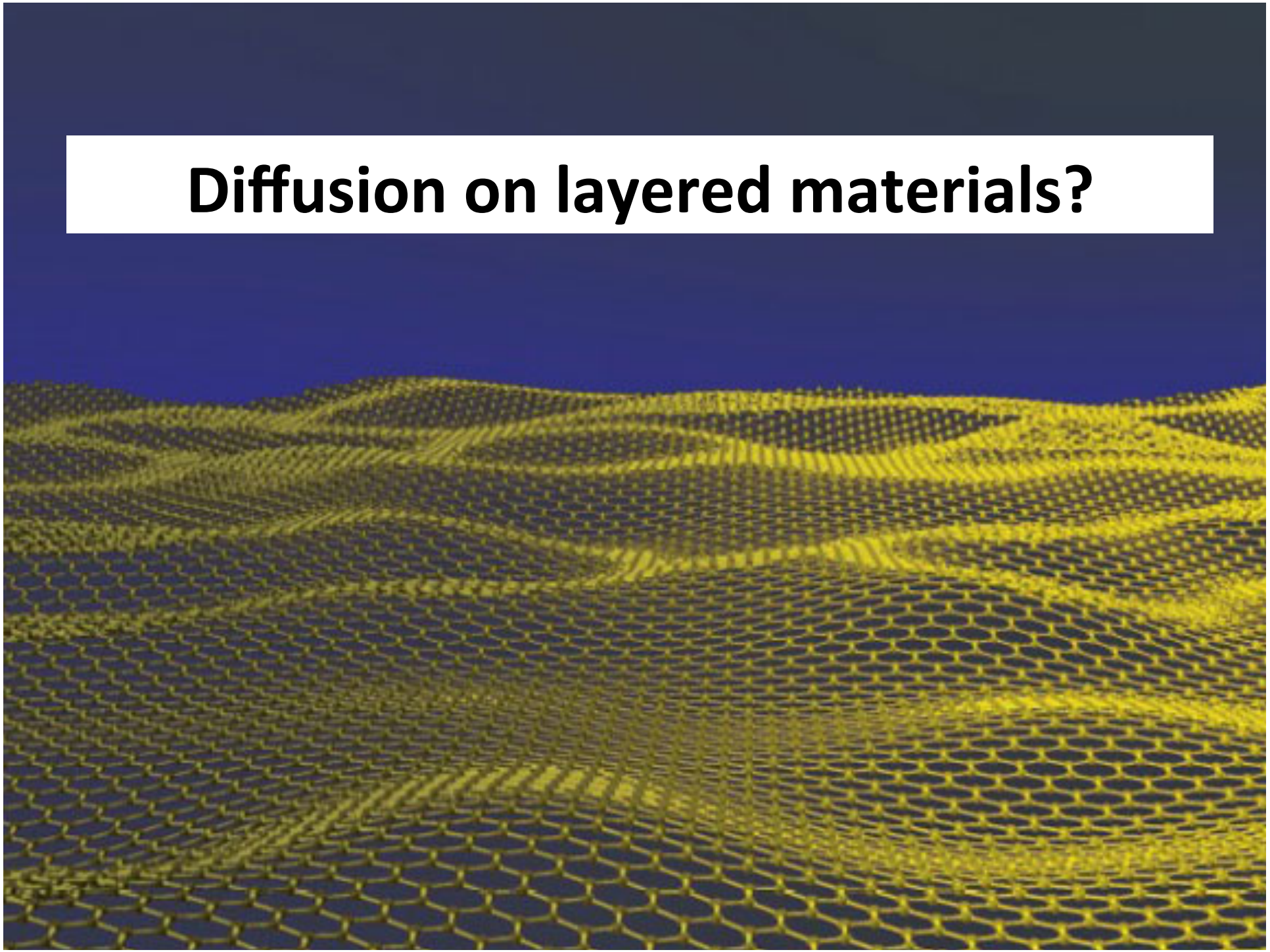
# Wet carbon and h-BN interfaces are interesting & technologically important



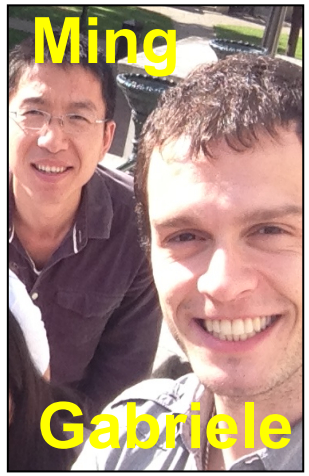



Ma et al. PRB 84, 003402 (2011); Chen et al. PCCP 15, 6344 (2013); Tocci et al. Nano Lett. 14, 6972 (2014); Al-Hamdani et al. J. Chem. Phys. 141, 18C530 (2014); Al-Hamdani et al. J. Chem. Phys. 142, 181101 (2015); Cox et al. J. Chem. Phys. 142, 184705 (2015); Ma et al. Nature Mater (in press)

# Diffusion on layered materials?

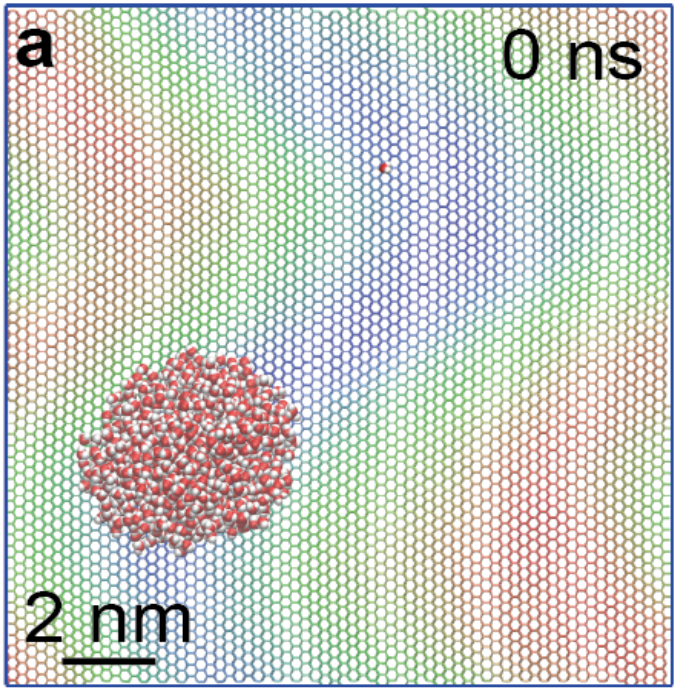


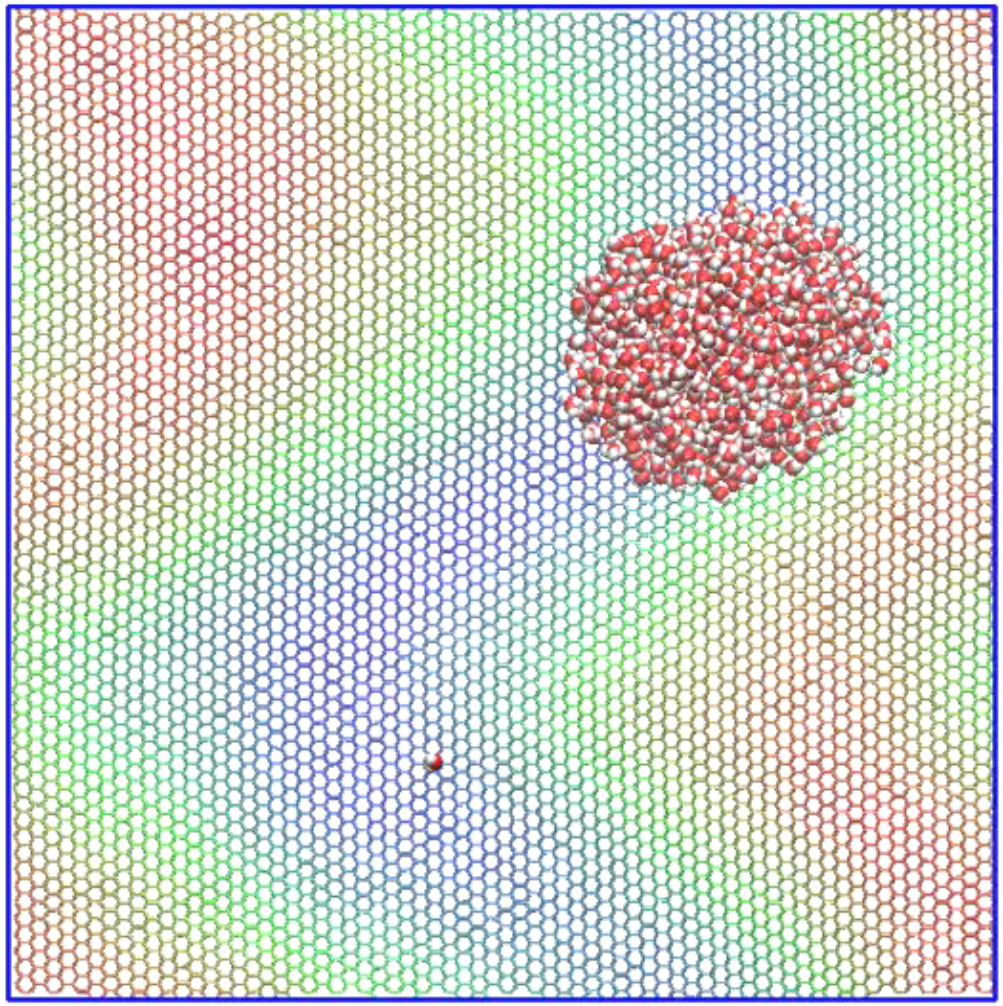
# Water nano-droplets on free-standing graphene



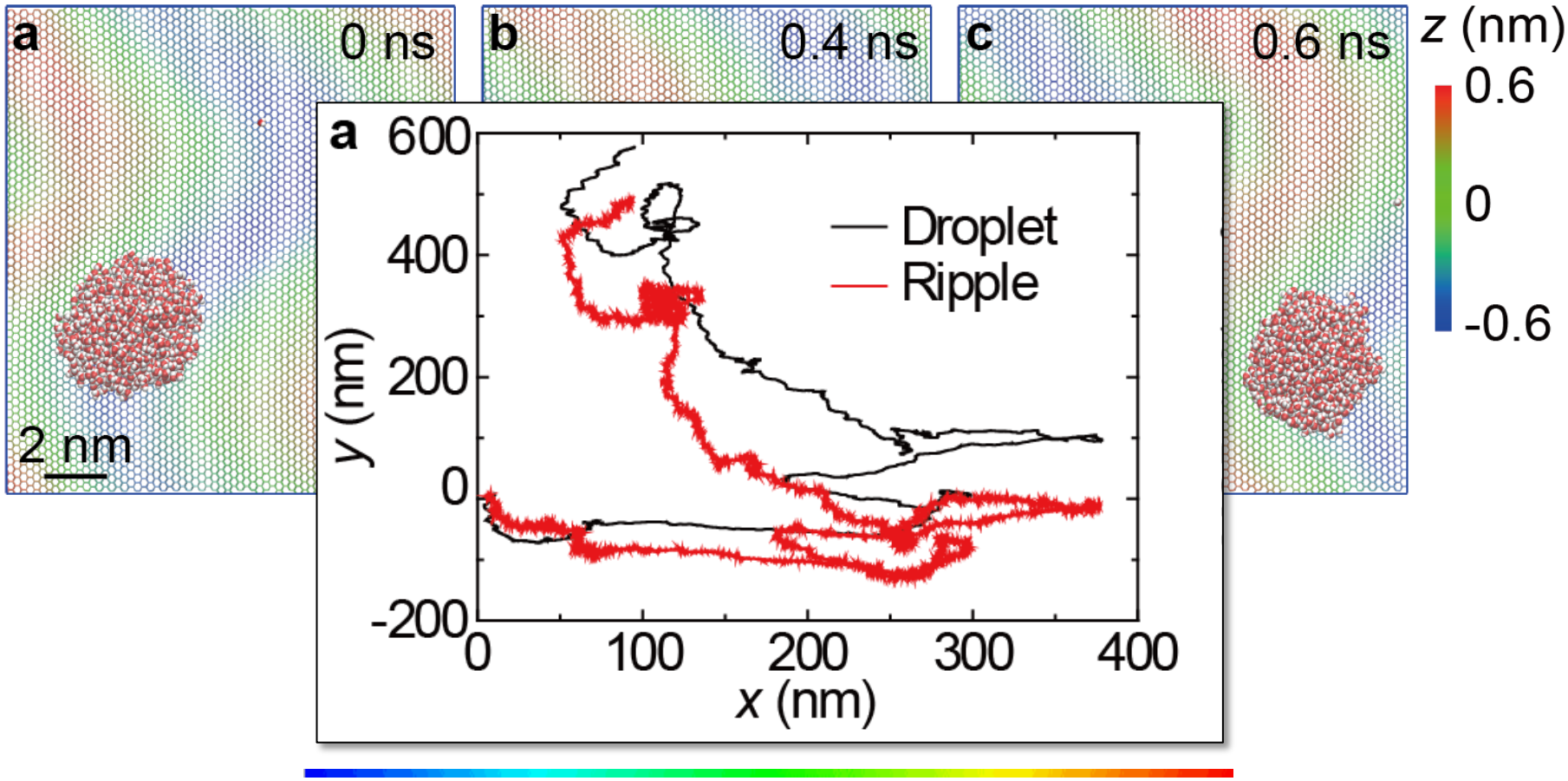

- Empirical potentials (T1P4P/2005 (water); Dreiding (carbon); Lennard Jones fitted to Quantum Monte Carlo (QMC)* for water-carbon
- 50+ ns trajectories at room temp.
- Droplets in the 2 nm (~100 waters) to 17 nm (~30,000 waters)

*Ma et al PRB 84, 003402 (2011)





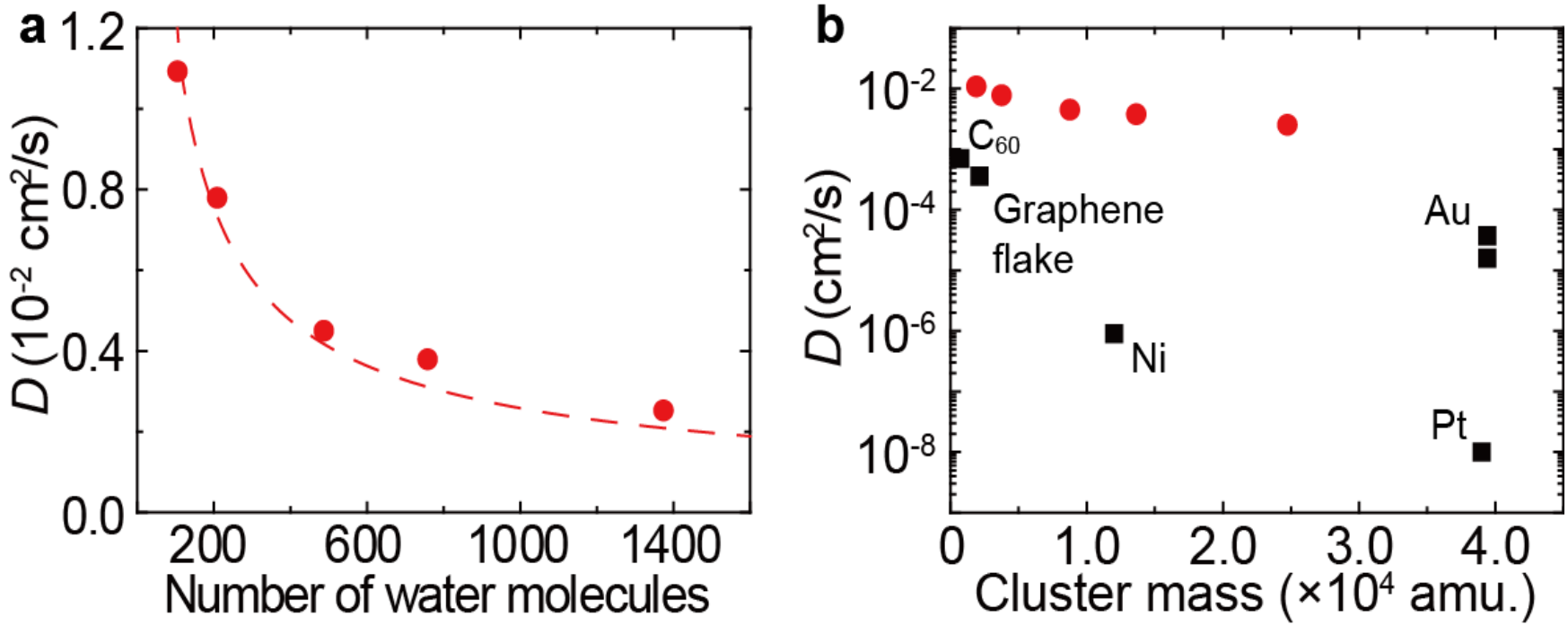
# Water droplets – surfing the waves




Ma et al. Nature Mater (in press)

Calculations: Ming Ma

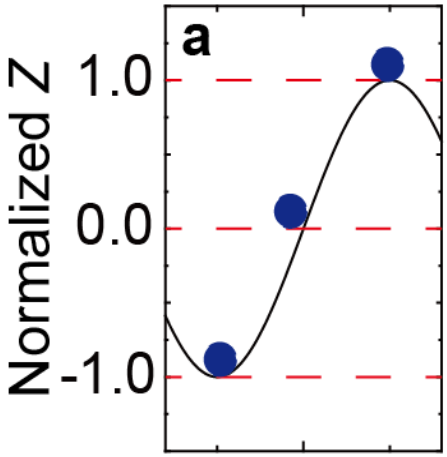
# Fast, size dependent diffusion




Ma et al. Nature Mater (in press)

Calculations: Ming Ma

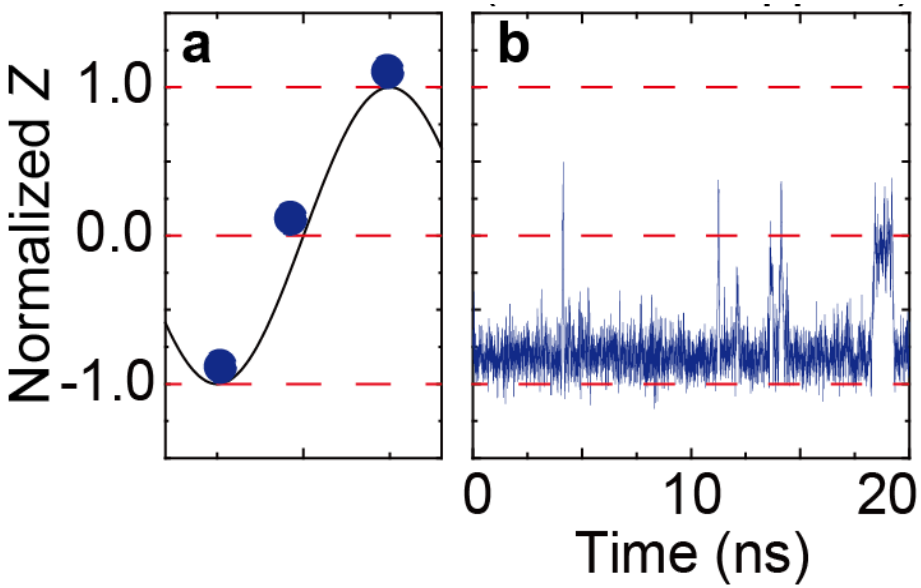
# To surf or not to surf? Controllable diffusion




Calculations: Ming Ma

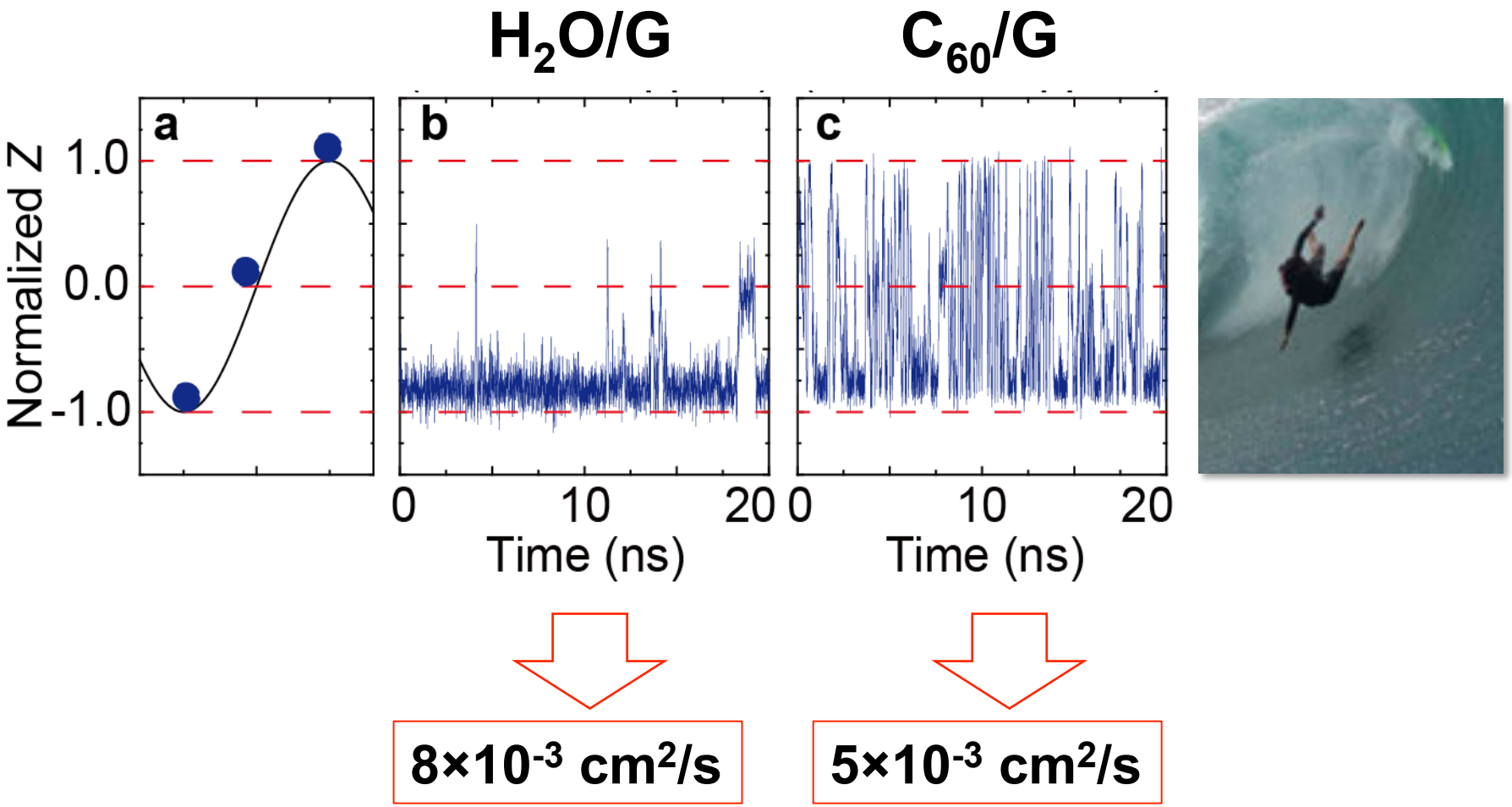
# To surf or not to surf? Controllable diffusion

$H_2O$/G



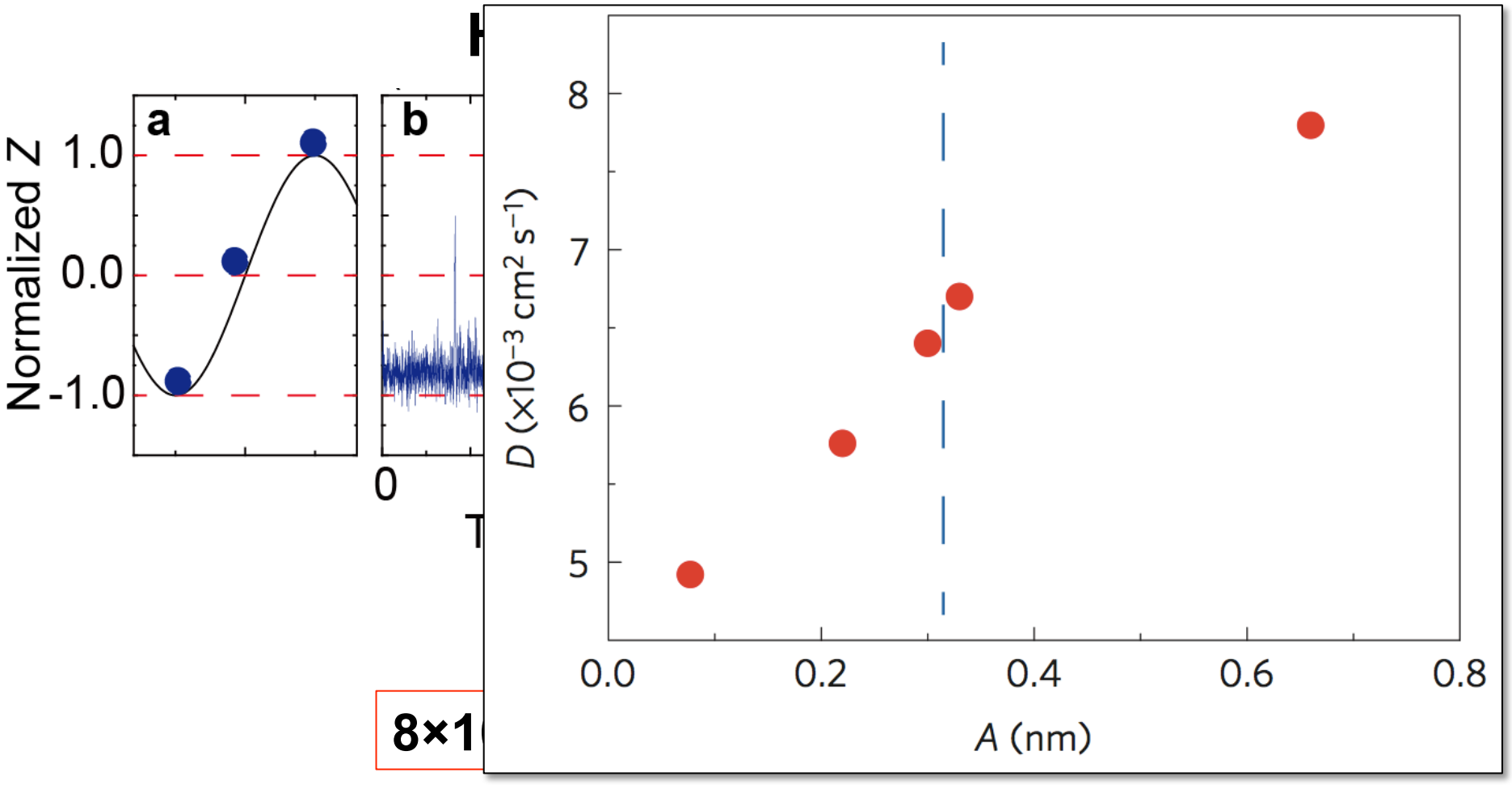

$8 \times 10^{-3}$ cm$^2$/s

# To surf or not to surf? Controllable diffusion




Calculations: Ming Ma

# To surf or not to surf? Controllable diffusion

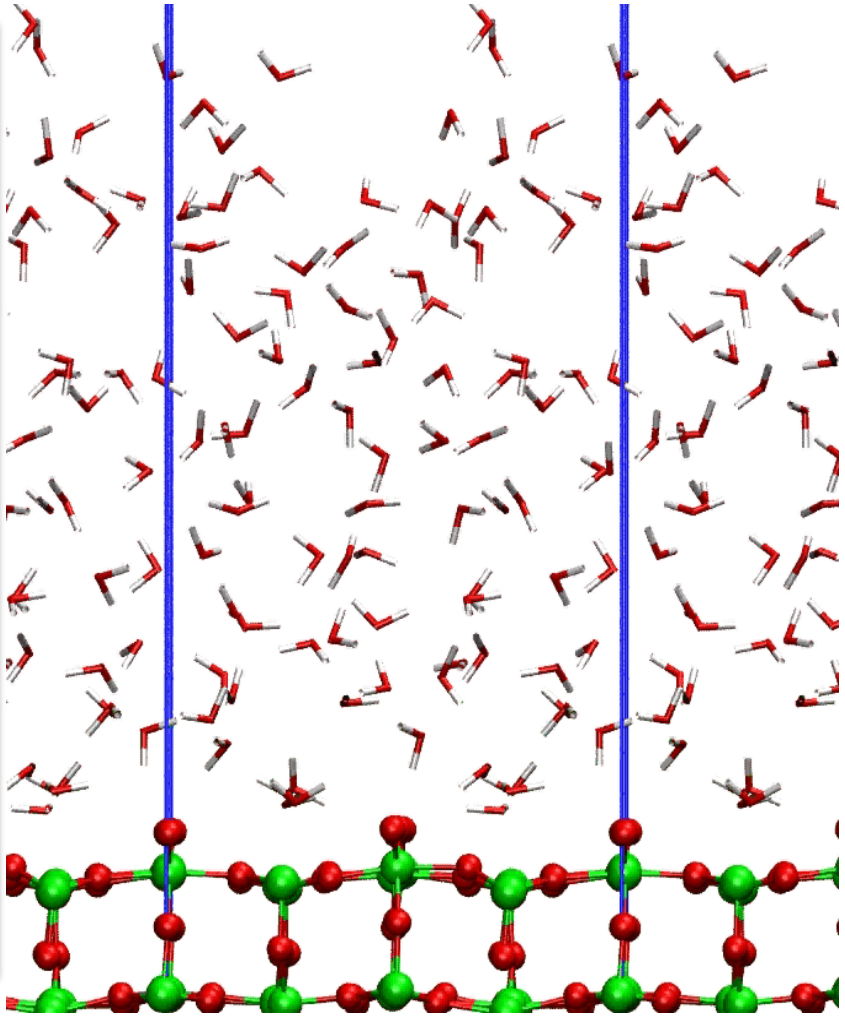



Calculations: Ming Ma

# Water/solid interfaces with ab initio MD

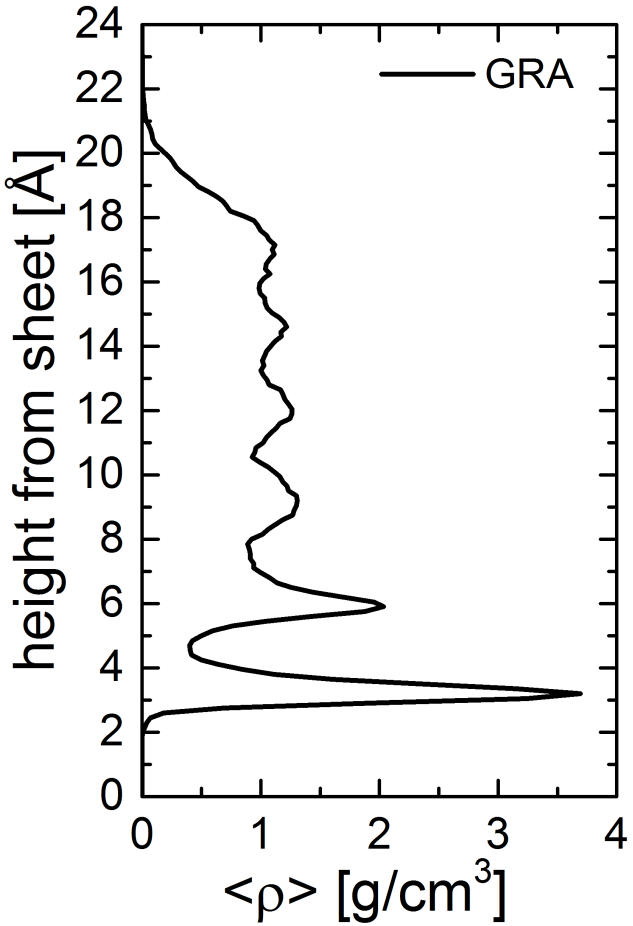
*Generic Questions on model systems:*

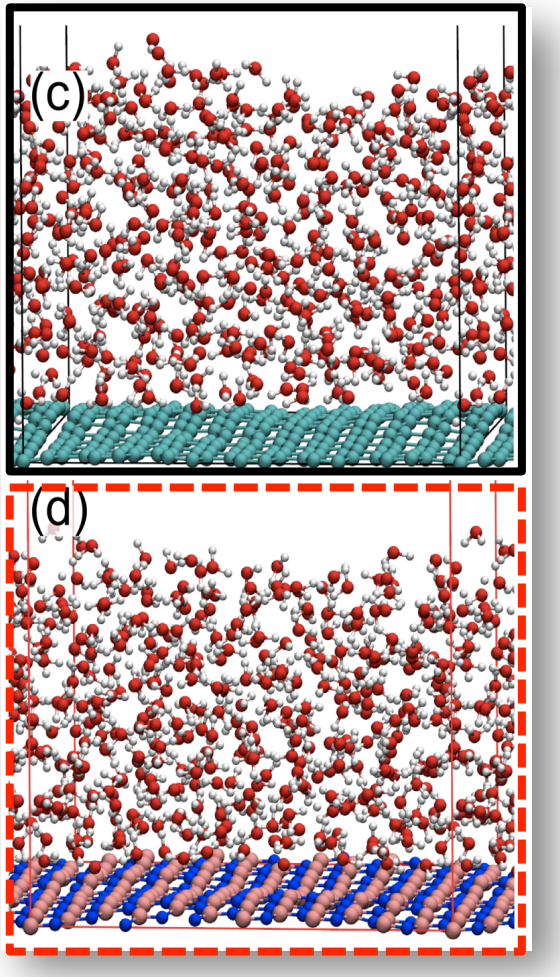
- How does the structure and dynamics change upon going beyond the first monolayer?
- **How does water structure (wetting) relate to friction?**
- How does the solvent alter the level of dissociation?
- What role does the solvent play in chemistry, e.g. dissolution?



[a]VandeVondele et al., Comp. Phys. Comm. 167, 103 (2005)

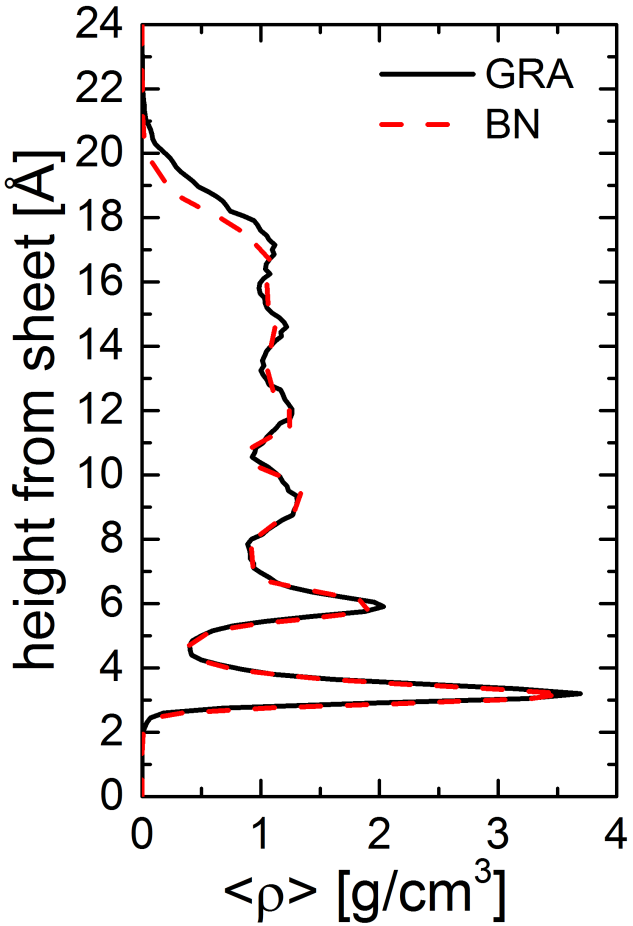
# Structure of water on graphene and BN

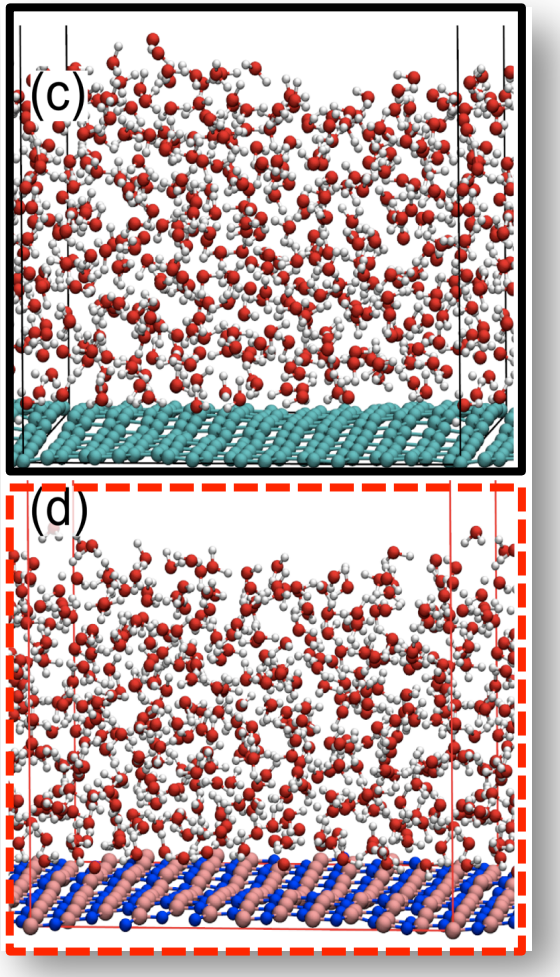



Tocci, Joly, Michaelides, Nano Lett 14, 6872 (2014)

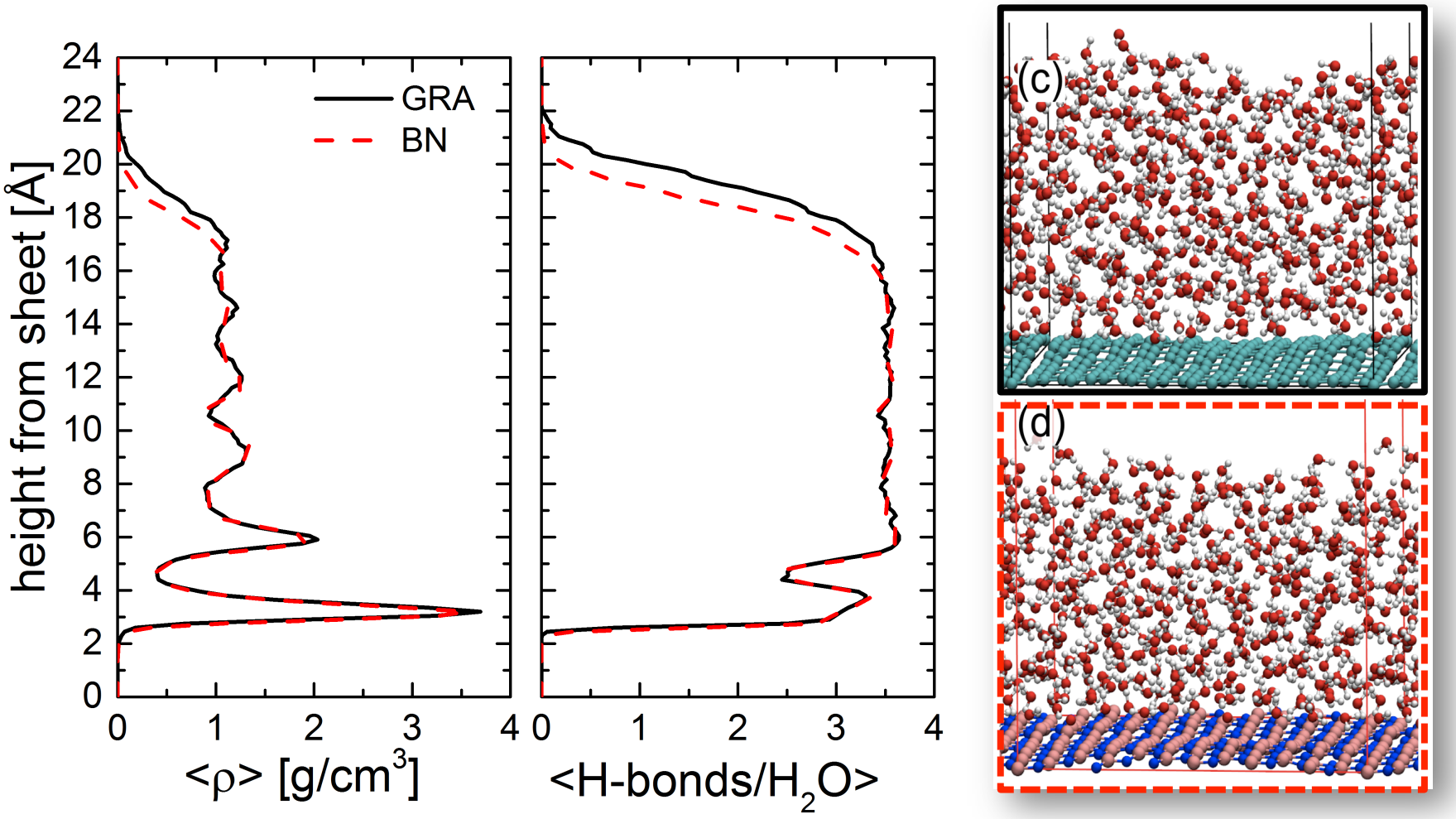
# Structure of water on graphene and BN



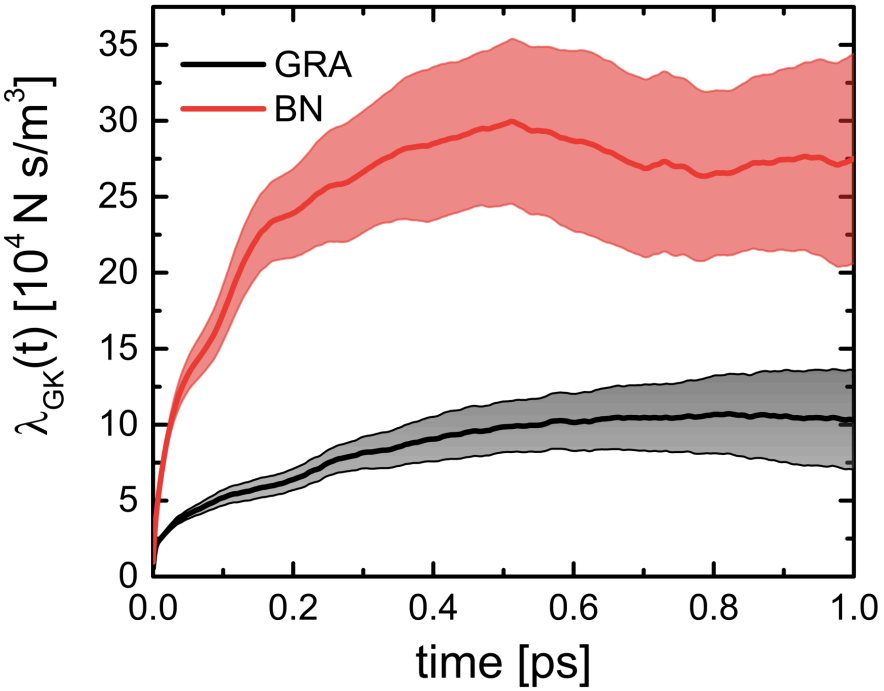

Tocci, Joly, Michaelides, Nano Lett 14, 6872 (2014)

# Structure of water on graphene and BN

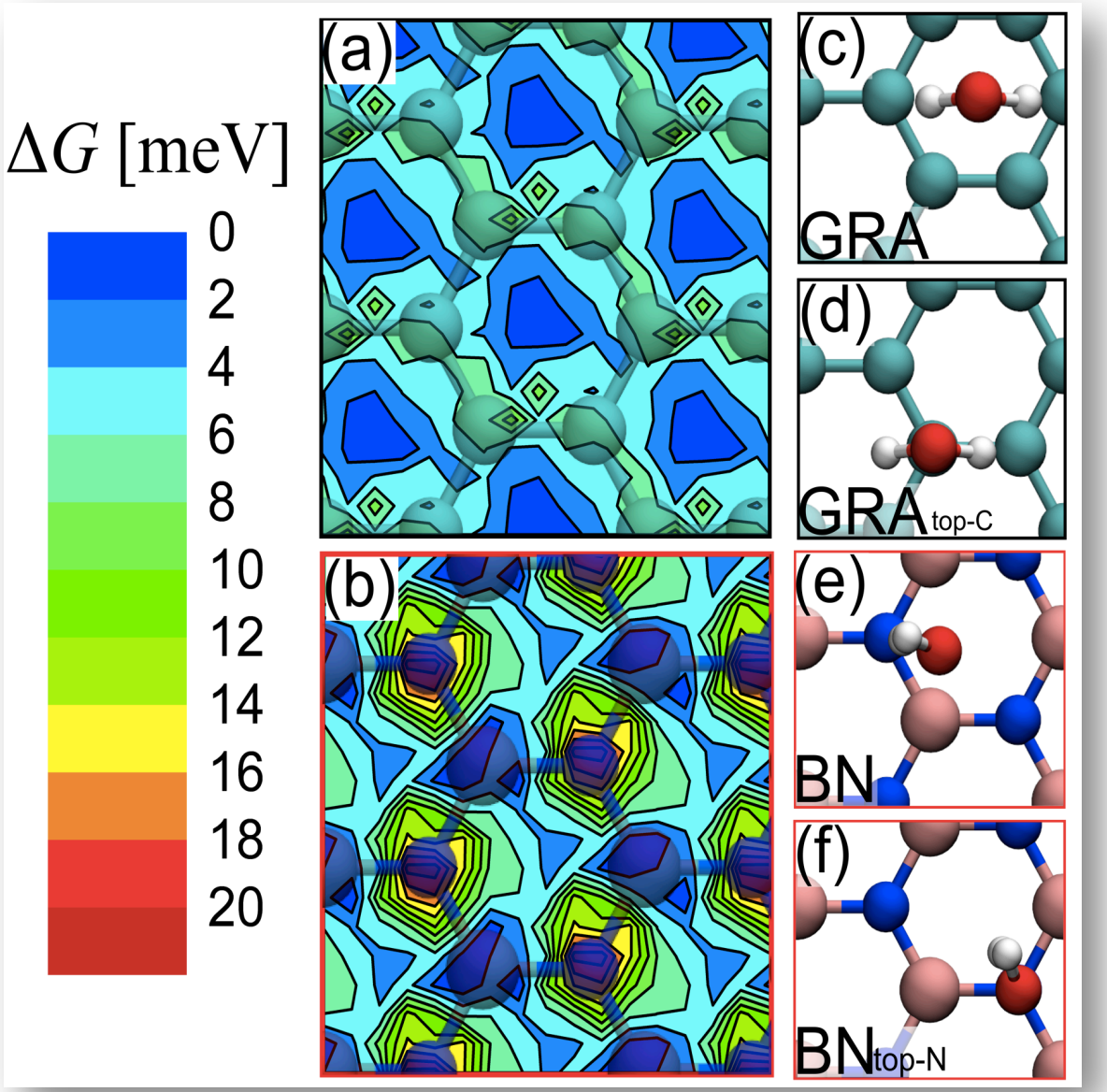



Tocci, Joly, Michaelides, Nano Lett 14, 6872 (2014)

# Dynamics: the Friction Coefficient




$$\lambda = \frac{1}{Ak_BT}\int_0^\infty dt\,\langle F(t)F(0)\rangle$$




# Why is the friction larger on BN?

- very small differences in free energy translate into large differences in friction

# Conclusions

- Water/solid interfaces are ubiquitous & challenging
- Water droplets can “surf” on graphene
- Very different friction of water on graphene compared to h-BN despite similar structure
- Clear distinction between “reactive” and “non-reactive” defects

Papers & More:
www.chem.ucl.ac.uk/ice


erc

THE THOMAS YOUNG CENTRE
TyC