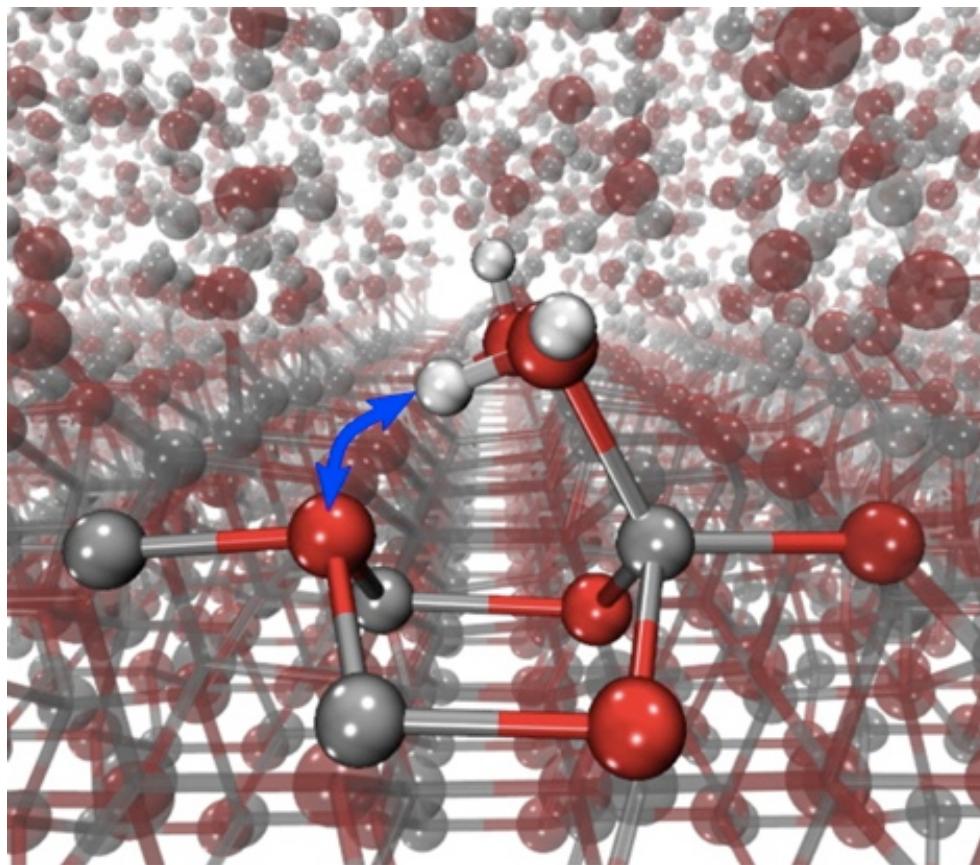


Ab-initio Molecular Dynamics of liquid/solid interfaces with CP2K

Gabriele Tocci

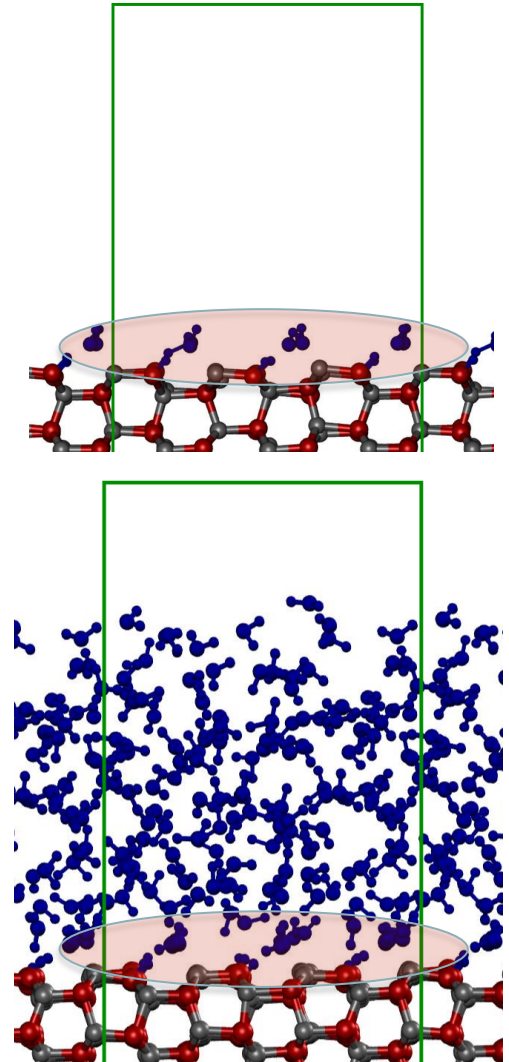
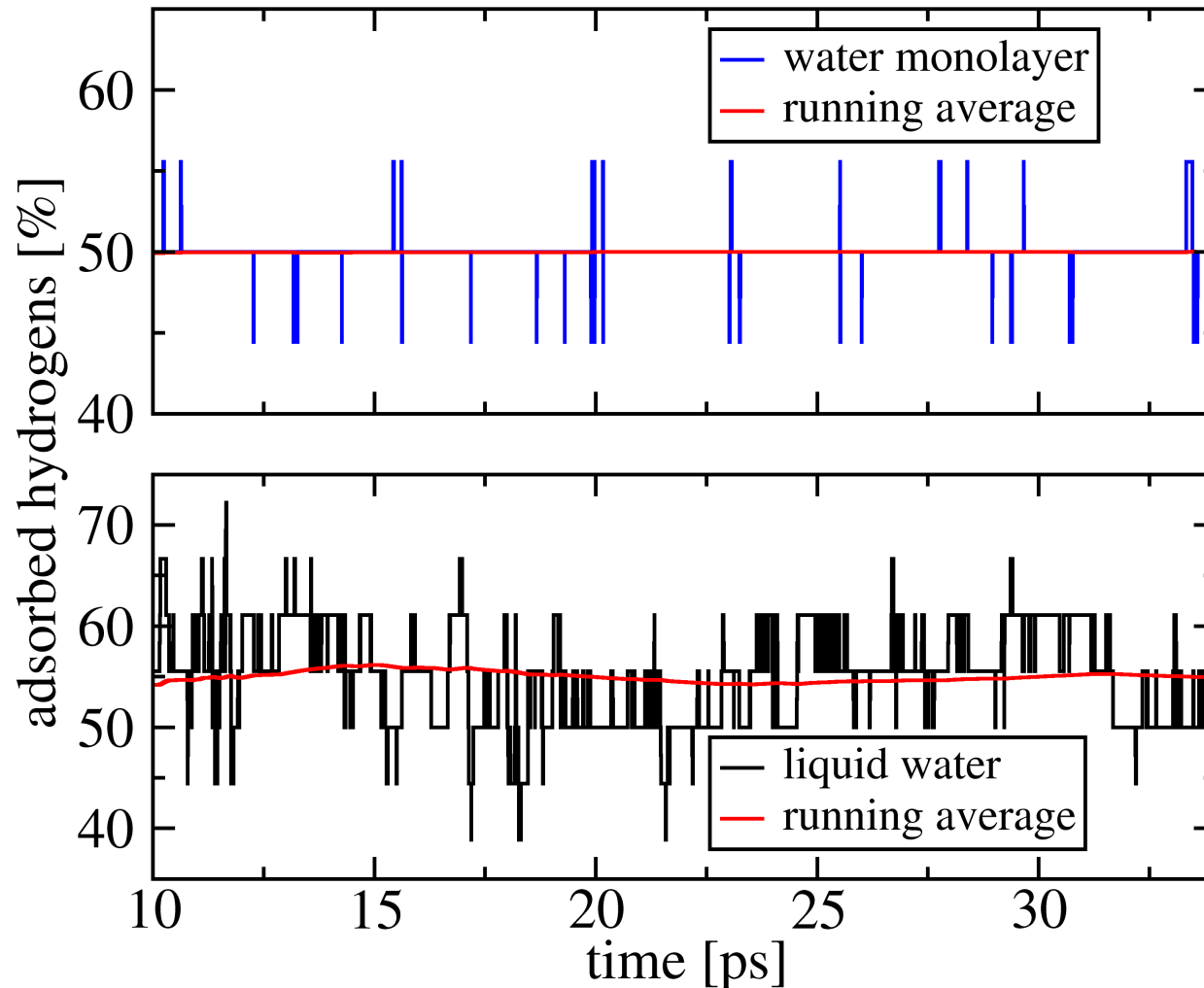
Angelos Michaelides



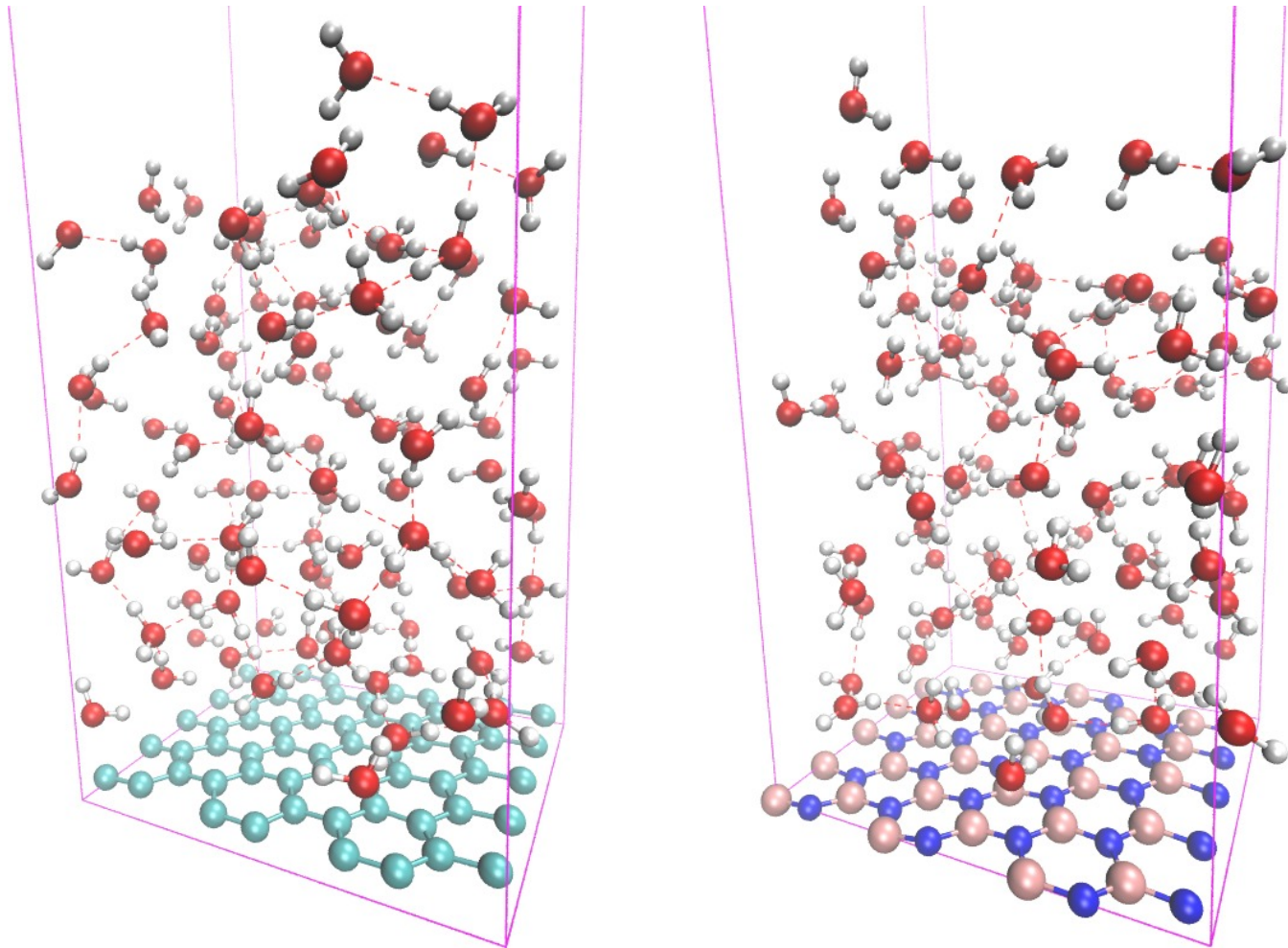
G. Tocci, A. Michaelides, *J. Phys. Chem. Lett.*, **2014**, DOI: 10.1021/jz402646c

Proton transfer dynamics at the water/ZnO interface

- AIMD of a water monolayer and liquid water on ZnO(10 $\bar{1}$ 0)



Structure and Dynamics at the Water/Graphene and Water/BN Interfaces



Courtesy of Laurent Joly