

Supplementary Information for:
Wetting of water on hexagonal boron
nitride@Rh(111): A QM/MM model based on atomic
charges derived for nano-structured substrates

Dorothea Golze,* Jürg Hutter,* and Marcella Iannuzzi*

E-mail: dorothea.golze@chem.uzh.ch; hutter@chem.uzh.ch; marcella.iannuzzi@chem.uzh.ch

Table S1: RESP charges for boron and nitrogen atoms of the wire region of the pristine *h*-BN/Rh(111) obtained with different strengths β of the harmonic restraints. The charges have been restrained to the target values of 0.255 and -0.255 , respectively

	target value	β		
		0.01	0.001	0.0001
B4	0.255	0.239	0.211	0.201
N4	-0.255	-0.272	-0.302	-0.311
RRMS		0.61	0.14	0.02

*To whom correspondence should be addressed

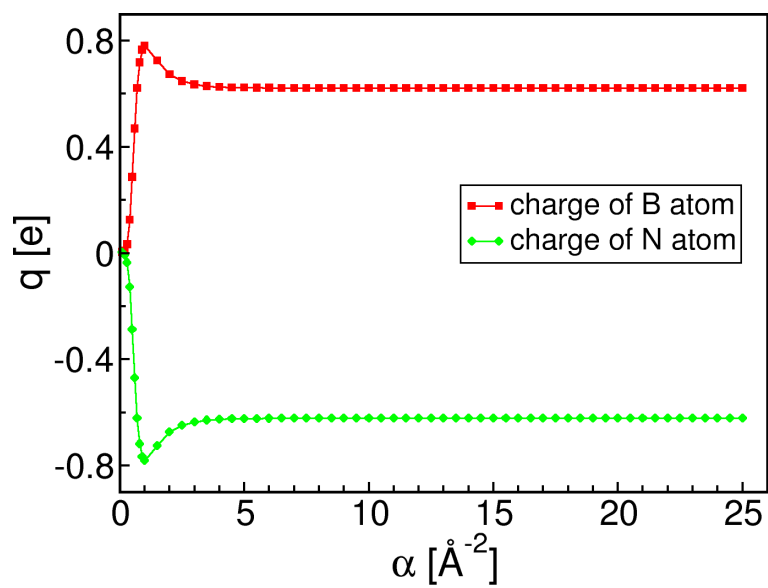


Figure S1: Dependence of the RESP charge q on the Gaussian width α . Charges fitted for a single h -BN sheet.

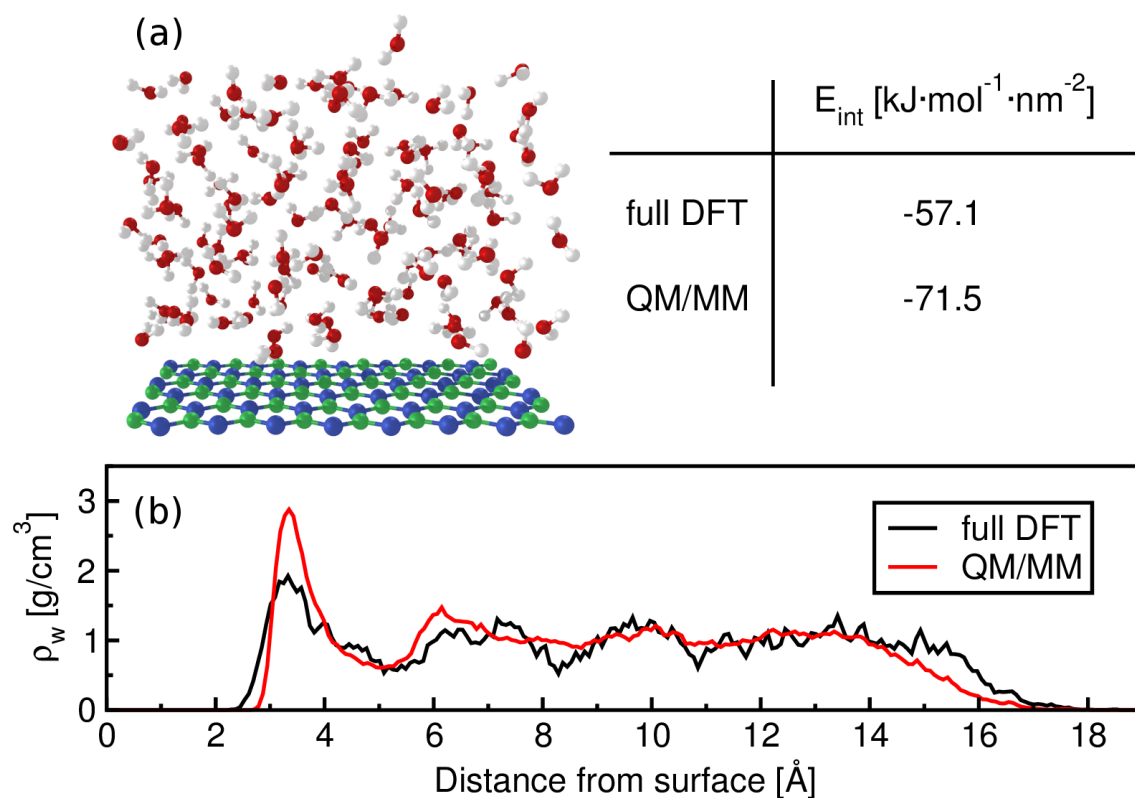


Figure S2: Results for a water slab on a free-standing BN layer. MD simulations have been carried out with full DFT meaning that the whole system is treated by DFT and with QM/MM treating BN and the interactions between water and BN at the MM level. For QM/MM, interactions between BN and water have been assumed to be of the Lennard-Jones type using the parameters given in Section 3.2. The setup of the calculations corresponds to the setup described in Section 3. (a) Snapshot of the simulation cell containing 120 water molecules and interaction energies E_{int} between water film and BN layer. (b) Plane-averaged water density ρ_w along the surface normal.

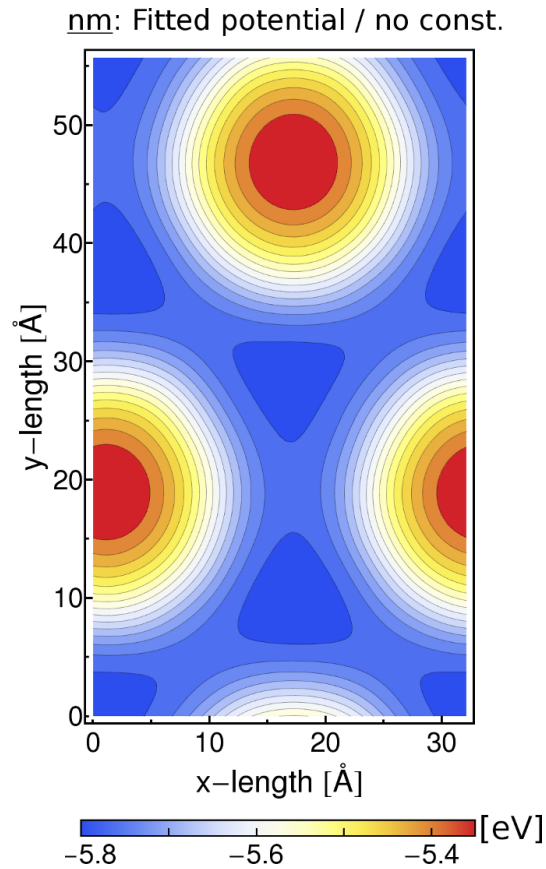


Figure S3: Electrostatic potential of nm at 4.8 \AA above the wire obtained by an unconstrained and unrestrained fit.

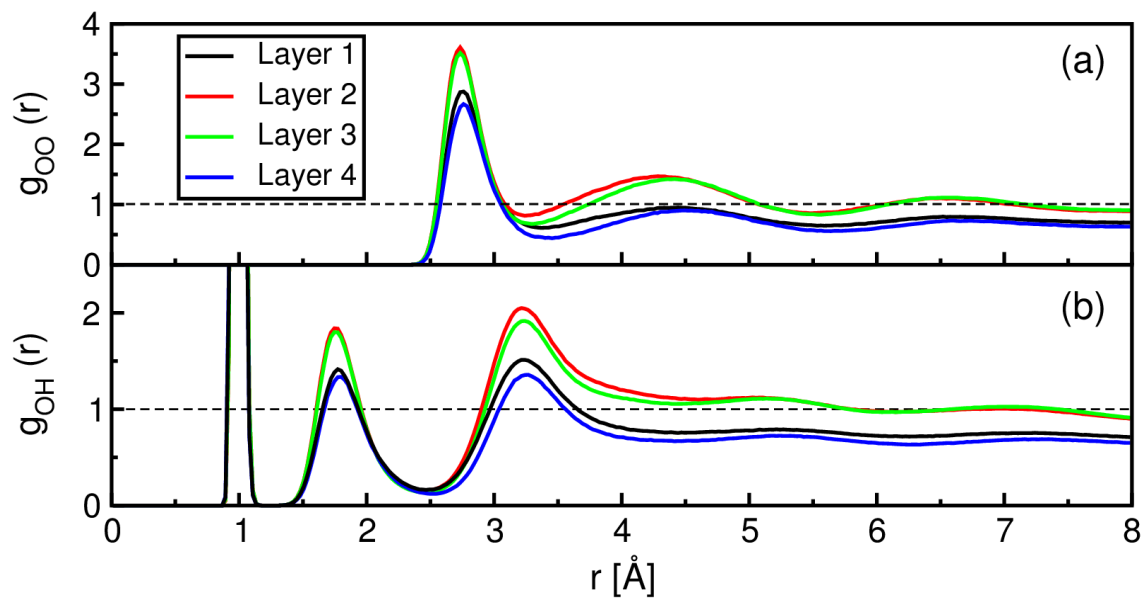


Figure S4: (a) Oxygen-oxygen and (b) oxygen-hydrogen RDFs for water/nm. The four different layers are defined as shown in Figure 5(c).

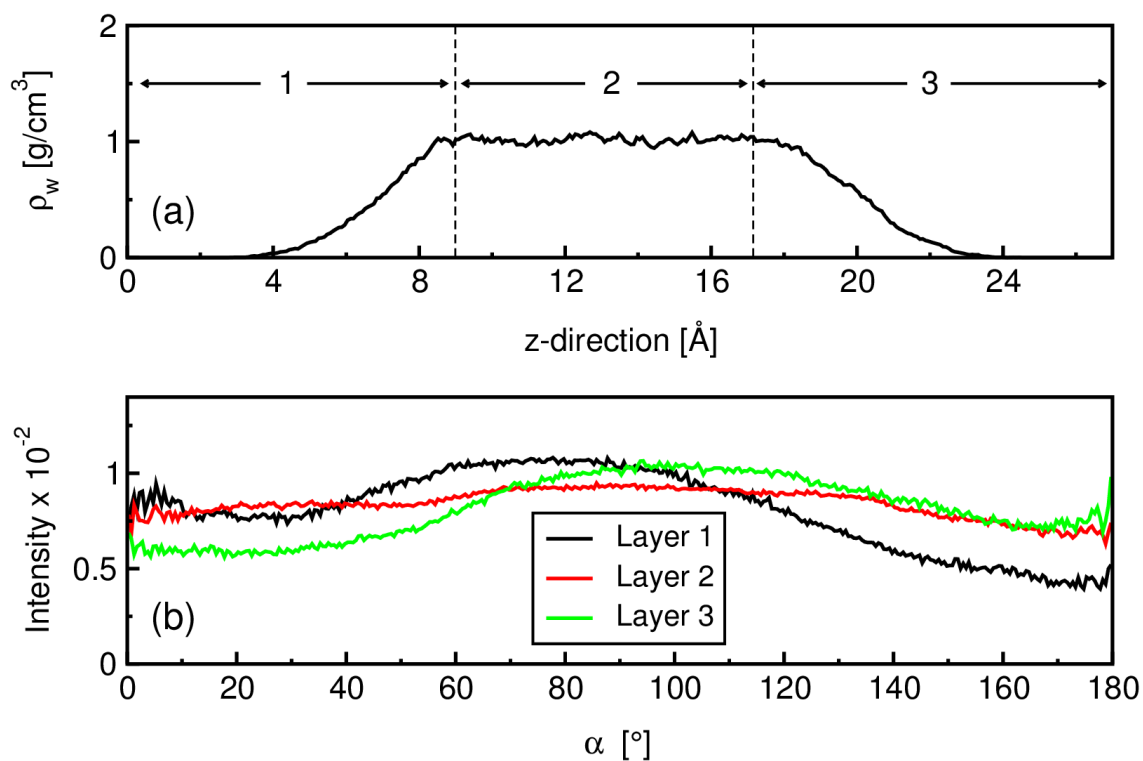


Figure S5: Results for the pure water slab. (a) Plane-averaged water density ρ_w along the z-direction which is perpendicular to the water-vacuum interface. The arrows indicate the division of the water film in three different layers. (b) Distribution of the orientation angle α for the three different layers.