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Ordering of confined water between metallic surfaces[1] ADRIEN POISSIER, MARIA V. FERNANDEZ-SERRA, Stony Brook University — It has been pointed out (PCCP 2010, Poissier et al.) that the hydrogen bonding type interaction occuring at water/metal interface makes the two type of interfacial water orderings (hydrophobic or hydrophilic overlayers) very close in energy. The most stable, hydrophobic, overlayer has very small net dipole moment perpendicular to the surface, while the least stable (in vacuum) hydrophilic interface has a large ($\approx 1.8D$) net dipole moment. First principles molecular dynamics simulations of liquid water confined between two Pd surfaces have been performed and structural and electronic water properties have been studied in detail. We show that water confinement in this situation results in a spontaneous symmetry breaking of the system, inducing an electric field across the liquid water slab. We discuss the origin of this spontaneous polarization and show its dependence with the confinement distance along the direction perpendicular to the planes of the surfaces.

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