

Abstract Submitted
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Charge induced hydrophobic/hydrophilic metallic surfaces LU-
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Brook University — Understanding the interaction of water-metal systems in an
atomic level is of fundamental importance in many areas, such as catalysis and ma-
terials science. We here present a detailed first-principles molecular dynamics study
of bulk water molecules confined within Pd(111) surfaces. We show that there is
a charge transfer between the substrate and the water inducing an asymmetry in
the order of water molecules at Pd surfaces. Our results show that the hydropho-
bic/hydrophilic character of a metallic surface depend on its charge, which can be
controlled by an applied voltage. We also propose a methodology to obtain the dipole
moment of each water molecule and show how they are affected by the substrate
induced polarization effects.

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