Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Water adsorption on non polar ZnO surfaces: from single molecules to multilayers STEPHANE KENMOE, P. ULRICH BIEDERMANN, Max-Planck Institute fuer Eisenforschung — The interface between water and ZnO plays an important role in many domains of technological relevance. Following the vital role of adsorbed water on substrate properties and the fascinating properties of interfacial water, there is a great interest in characterizing this interface. We use DFT to study the possible aggregation regimes that can form on the ZnO non-polar low-index (1010) and (1120) surfaces. We study the adsorption of water monomers, small water clusters like water dimers, water chains, ladder-like water structures, water thin films and water multilayers. Based on this, trends in binding energy as well as the binding mechanisms are analyzed to understand the driving forces and the nature of the fundamental interactions that stabilize the adsorbed layers.

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Date submitted: 14 Nov 2014 Electronic form version 1.4