

Abstract Submitted
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Autocatalytic dissociation of water at stepped transition metal surfaces RENGIN PEKOEZ, SWENJA WOERNER, Max Planck Institute for Polymer Research, Germany, LUCA M. GHIRINGHELLI, Fritz Haber Institute, Germany, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Germany — By means of density functional theory calculations, we investigate the adsorption and dissociation of water clusters on flat and stepped surfaces of several transition metals: Rh, Ir, Pd, Pt, and Ru. We find that water binds preferentially to the edge of the steps than to terrace sites, so that isolated clusters or one-dimensional water wires can be isolated by differential desorption. The enhanced reactivity of metal atoms at the step edge and the cooperative effect of hydrogen bonding enhance the chances of partial dissociation of water clusters on stepped surfaces. For example, water dissociation on Pt and Ir surface turns from endothermic at terraces to exothermic at steps. The interpretation of water dissociation is achieved by analyzing changes in the electronic structure of both water and metals, especially focusing on the interaction between the lone-pair electrons of water and the d-band of the metals [1]. The shift in the energetics of water dissociation at steps is expected to play a prominent role in catalysis and fuel cells reactions, as the density of steps at surfaces could be an additional parameter to design more efficient anode materials or catalytic substrates.

[1] D. Donadio, L.M. Ghiringhelli, and L. Delle Site, *J. Am. Chem. Soc.* 134, 19217 (2012).

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