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PII: S1572-6657(17)30623-9
DOI: doi: 10.1016/j.jelechem.2017.09.002
Reference: JEAC 3496

To appear in: *Journal of Electroanalytical Chemistry*

Received date: 8 June 2017
Revised date: 29 August 2017
Accepted date: 3 September 2017

Please cite this article as: Jiabo Le, Angel Cuesta, Jun Cheng, The Structure of Metal-water Interface at the Potential of Zero Charge from Density Functional Theory-based Molecular Dynamics, *Journal of Electroanalytical Chemistry* (2017), doi: 10.1016/j.jelechem.2017.09.002

The Structure of Metal-water Interface at the Potential of Zero Charge from Density Functional Theory-based Molecular Dynamics

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(Dated: September 6, 2017)

Abstract

We simulated a series of transition metal-water interfaces, namely Pt(111), Au(111), Pd(111) and Ag(111), by density functional theory based molecular dynamics, and found some common structural features for the surface water on different transition metal surfaces. Firstly, there exists a pronounced adsorption layer within ∼5 Å distance from metal surfaces , in which three main water species with different orientations (watA, watB-down and watB-up) could be identified. WatA and watB-down show a lower degree of hydrogen bonding, due to their interaction with the metal surface via one of the lone pairs of the oxygen atoms and via one of their H atoms, respectively. While, watB-up has an almost full coordination shell, indicating it not only forms hydrogen bonds in the adsorption layer, but also with the non-surface water. As expected, the honeycomb-like bilayer model used as the starting point of the simulation was destructed into irregular patterns after ∼10 ps of molecular dynamics simulations, and the surface water coverage concomitantly increases from 0.66 ML to ∼0.8 ML.