

**Impact of adsorbates on water-surface interaction:  
A density functional theory study**

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Abstract:

Interaction of water with a surface has been studied extensively, because it has implications for various fields ranging from daily life to science and technology, including wetting, lubrication, corrosion, heterogeneous catalysis, and electrochemistry. In many theoretical studies of water on metal surfaces, only clean surfaces were considered, and less attention has been paid for the interaction of water with adsorbates and that between adsorbates. However, these interactions are particularly important in electrochemistry, as they are directly related to heterogeneous catalytic reactions at electrode/electrolyte interfaces. In this talk, I will introduce density functional theory study of interactions between water and metal surfaces with and without adsorbate and discuss how the specific adsorbates modify the water-surface interactions. I will discuss the implication to the electrochemistry and how the surface science approach helps to understand the complex electrochemical interfaces.

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Reference:

- I. Hamada and Y. Morikawa, J. Chem. Phys. 134, 154701 (2011).*  
*T. Kumagai, M. Kaizu, H. Okuyama, S. Hatta, T. Aruga, I. Hamada, Y. Morikawa, Phys. Rev. B 81, 045402 (2010).*  
*I. Hamada, T. Kumagai, A. Shiotari, H. Okuyama, S. Hatta, and T. Aruga, Phys. Rev. B 86, 075432 (2012).*