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Water monolayers on metals – a new framework[1]

PETER J. FEIBELMAN, Sandia National Laboratories

The first wetting layer on a solid embodies the boundary condition for water transport along its surface, is the template for ice nucleation, and governs aqueous surface chemistry. Today's talk is focused on the wetting of close-packed, precious metal surfaces, which are both relatively easily prepared, and susceptible to study by a host of surface science techniques. For decades, wetting layers on such surfaces have been thought to be "ice-like" – strained into registry with the metal lattice, but otherwise like the layers that stack to form the naturally occurring crystal, ice Ih. Interpretations of STM images of periodic wetting layers on Pt(111) [1], of TPD [2], and of IR absorption spectra [3] contradict the "ice-like" picture, but submit to a common, physics-based and DFT-supported interpretation. It is that several ice-like hexagonal rings of H_2O molecules, per repeated cell, are replaced by pentagons and heptagons, allowing a compact subset of H_2O's, with planes parallel to the metal surface, to approach the metal exceptionally closely and to anchor the wetting layer strongly to it. This motif, amounting to formation of energetically favorable di-interstitial "defects," appears to be general; similar molecular arrangements account for what we know experimentally (and, largely, could not previously explain) of water bonding to Ni, Ru, and Pd close-packed surfaces.

[1] S. Nie, P. J. Feibelman, N.C. Bartelt, and K. Thürmer, Phys. Rev. Lett. **105**, 026102(2010).
[2] P. J. Feibelman, N.C. Bartelt, S. Nie, and K. Thürmer. J. Chem. Phys. **133**, 154703(2010).
[3] P. J. Feibelman, G. A. Kimmel, B. D. Kay, N. Petrik, R. S. Smith and T. Zubkov, unpublished.

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