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Interactions of oxygen and hydrogen on Pd(111) surface[1] DENIS DEMCHENKO, Virginia Commonwealth University, SACHA GOMEZ, MIQUEL SALMERON, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The coadsorption and interactions of oxygen and hydrogen on Pd(111) was studied by scanning tunneling microscopy and density functional theory calculations. In the absence of hydrogen oxygen forms a (2×2) ordered structure. Coadsorption of hydrogen leads to a structural transformation from the (2×2) to a $(\sqrt{3} \times \sqrt{3})$R30° structure. In addition, hydrogen enhances the mobility of oxygen. To explain these observations, the interaction of oxygen and hydrogen on Pd(111) was studied within the density functional theory. In agreement with the experiment the calculations find a total energy minimum for the oxygen (2×2) structure. The interaction between H and O atoms was found to be repulsive and short ranged, leading to the compression of the O islands from (2×2) to $(\sqrt{3}\times\sqrt{3})$R30° ordered structure at high H coverage. The computed energy barriers for the oxygen diffusion were found to be reduced due to the coadsorption of hydrogen, in agreement with the experimentally observed enhancement of oxygen mobility. The calculations also support the finding that at low temperatures the water formation reaction does not occur on Pd(111).

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