

Water-Related Adsorbates on Stepped Platinum Surfaces

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Chapter 6

Notes regarding the Supporting Information

• Chapter 2:

The supporting information for chapter 2 contains a full list of adsorption geometry information, adsorption energies and ZPE as well as vibrational entropy correction terms. Furthermore, we give information regarding the convergence of the model surfaces.

The supporting information is available online at the online repository of the Journal of Chemical Physics. ftp://ftp.aip.org/epaps/journ_chem_phys/E-JCPSA6-140-043413/

• Chapter 3:

The supporting information for this chapter contains the full set of adsorption geometries and energies for all tested adsorption structures of water in this study. Additionally, we give account for the calculated ZPE and vibrational entropy terms of each structure.

The supporting information is available online at the repository of the journal Physical Chemistry Chemical Physics at http://www.rsc.org/suppdata/c5/cp/c5cp04468e/c5cp04468e1.pdf

• Chapter 4:

The supporting information for chapter 4 contains a set of 5 additional STM images that we analyzed to help elucidate and confirm the adsorption structure present on the surfaces. Additionally, we give a full account of all tested adsorption structures, their adsorption energies as well as the ZPE and vibrational entropy contributions to the free energy.

The supporting information will be available online as part of the publication of the article on which the chapter is based. Until that point in time the supporting material is available online at https://www.dropbox.com/s/ywbpfrm4mo8h0ix/Supplemental-Material.pdf?dl=0.