

Supporting Information to
Free energy assessment of water structures and their
dissociation on Ru(0001)

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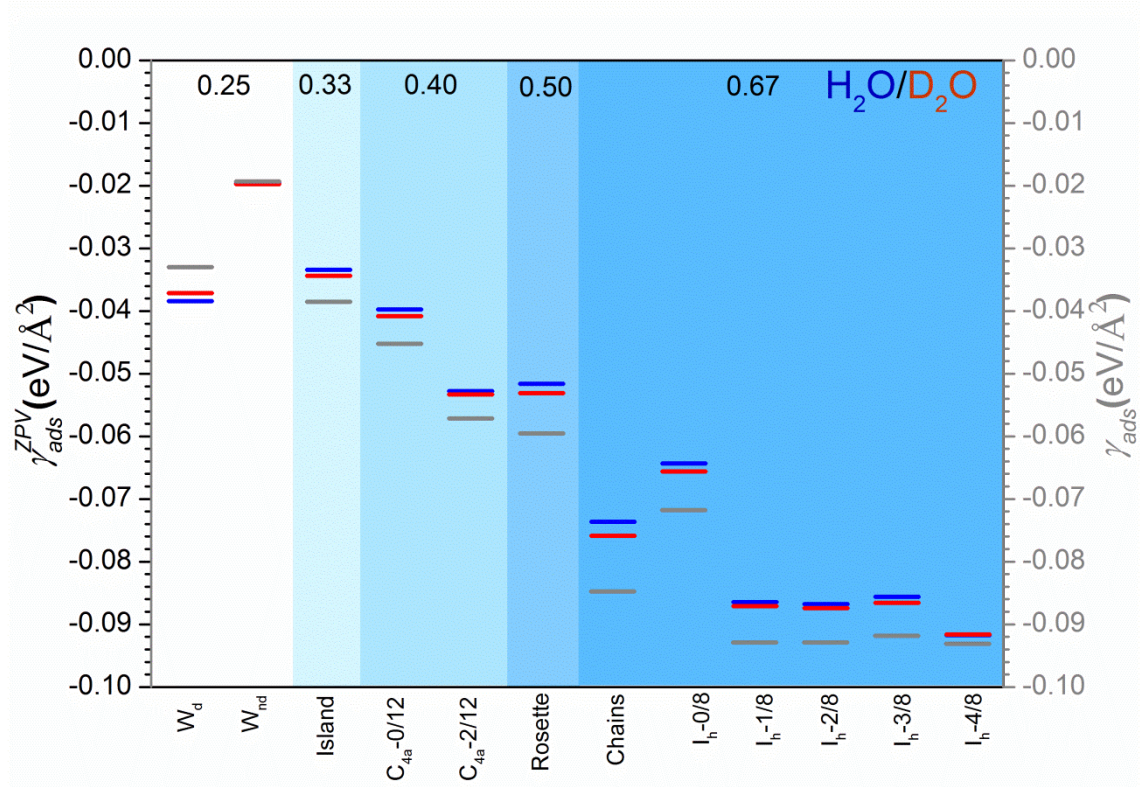


Figure S1: γ_{ads}^{ZPV} in $eV \cdot \text{\AA}^{-2}$ scale on the left, for the adsorption of H_2O (blue) and D_2O (red). γ_{ads} in $eV \cdot \text{\AA}^{-2}$ is presented in grey to be read on the right. Considered systems are described by their coverage (top) in ML and presented for: W_d single dissociated water; W_{nd} molecular water; Island; the new chains reported by Salmeron *et al.*¹⁷: $C_{4a-2/12}$ and $C_{4a-0/12}$; Rosette; Chains and different I_h -like models with different amount of dissociated molecules.

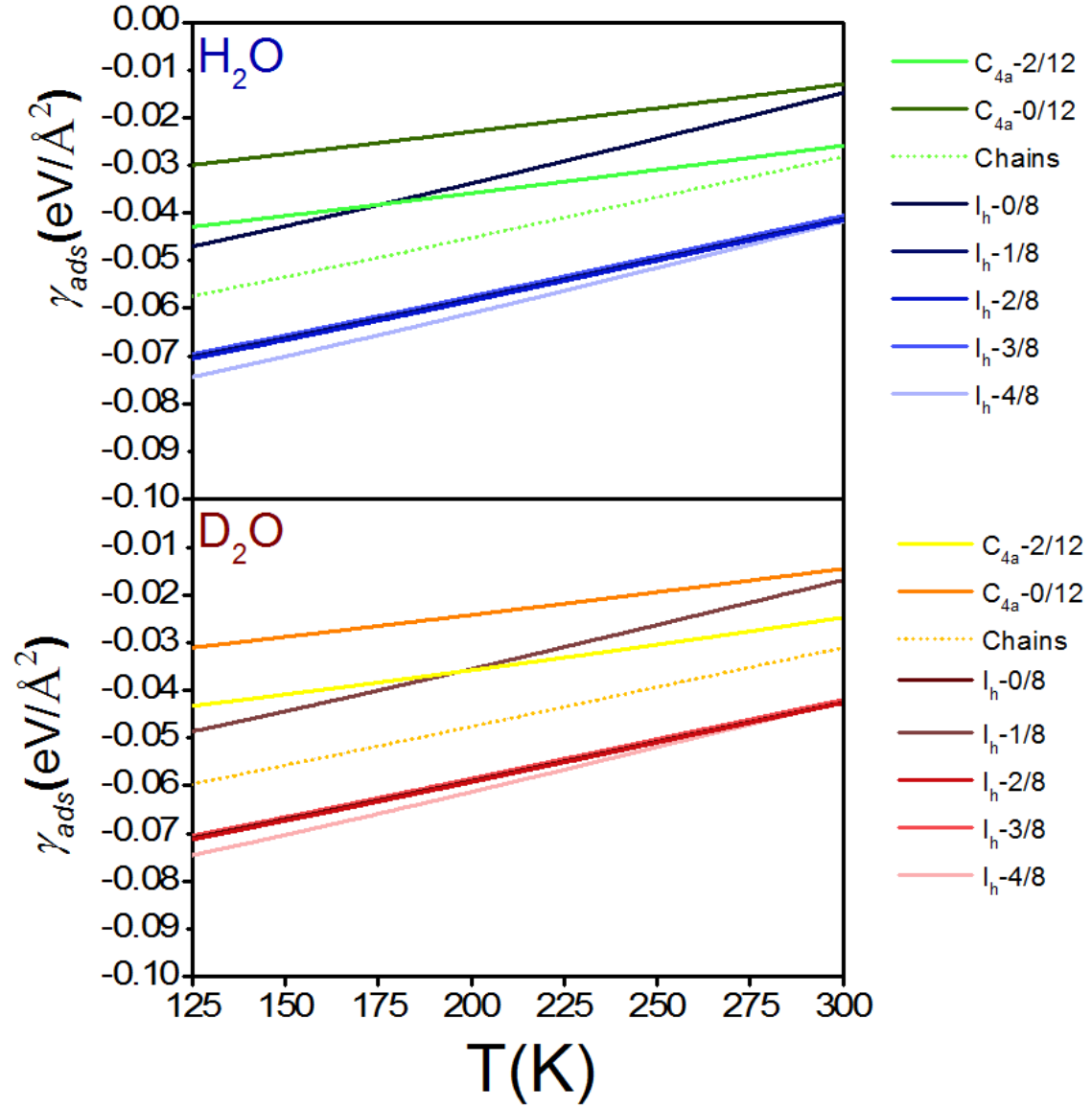


Figure S2: γ_{ads} in $\text{eV}\cdot\text{\AA}^{-2}$ for H_2O and D_2O , as a function of temperature for the different ensembles in the present work.

The Energies and Cartesian coordinates of the geometry optimized structures in this work are:

1-I_h-0/8

E= -.16356586E+03 eV

Bilayer/Ru0001

1.0

+4.7300000000 +0.0000000000 +0.0000000000
+2.3650000000 +4.0963000000 +0.0000000000
+0.0000000000 +0.0000000000 +32.1264000000

Ru O H

15 2 4

Cartesian

+0.0000000000 +0.0000000000 +0.0000000000
+2.3651150000 +1.3655000001 +0.0000000000
+4.7302310000 +2.7310000001 +0.0000000000
+3.1534929998 +2.7309889999 +2.1400000012
+3.1534930003 +0.0000110002 +2.1400000012
+0.7886089998 +1.3654889999 +2.1400000012
+0.0000000000 +0.0000000000 +4.2799999992
+2.3651150000 +1.3655000001 +4.2799999992
+4.7302310000 +2.7310000001 +4.2799999992
+3.1586619999 +2.7253600001 +6.4203280014
+5.5136740002 +4.0925769999 +6.4148949998
+0.7964100001 +1.3636850000 +6.4264079997
+2.3686339999 +4.0873059999 +8.4264109996
+2.3837440000 +1.3571200001 +8.5454200005
+4.7386190003 +2.7307050002 +8.4494779990
+0.3590669998 +0.0124380000 +11.5042369987
+2.7022089998 +1.3884389999 +11.0629040002
+2.6830649998 +3.1096589999 +11.5517709985
+0.6019459998 +0.1321319999 +10.5333169987
+1.9626339998 +0.8656369998 +11.4715920015
+3.5373949999 +0.8734269999 +11.2593029992

2-I_h-4/8

E= -.16398211E+03 eV

H2O/Ru0001-I_h-4/8

1.0

+4.7300000000 +0.0000000000 +0.0000000000
+2.3650000000 +4.0963000000 +0.0000000000
+0.0000000000 +0.0000000000 +32.1264000000

Ru O H

15 2 4

Cartesian

+0.0000000000 +0.0000000000 +0.0000000000
+2.3651153174 +1.3654999665 +0.0000000000
+4.7302306348 +2.7309999330 +0.0000000000
+3.1534934123 +2.7309890368 +2.1399999016
+3.1534934123 +0.0000108962 +2.1399999016
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+2.2917825120 +1.6956971706 +10.6343895698
+2.0800280039 +3.2280422749 +10.8496570651
+3.9766492365 +4.0157993251 +9.3294398219
+1.4805382470 +1.2209579756 +10.9252409307
+3.5878424890 +0.6306396645 +10.8476366094

3-I_h-1/8

E= -.26231505E+04

H2O/Ru0001-1/8

1.0

+18.9200000000 +0.0000000000 +0.0000000000
+9.4600000000 +16.3852000000 +0.0000000000
+0.0000000000 +0.0000000000 +32.1264000000

Ru O H

240 32 64

Cartesian

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+4.7302306641 +2.7309999477 +0.0000000000
+2.3650000000 +4.0963000000 +0.0000000000
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+21.2907474103 +9.9971080745 +10.6483672892
+21.0853423831 +12.6258807981 +11.4034170766
+23.5843431903 +13.7838402327 +10.6146693682
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4-Chains

E= -.65495268E+03eV

H2O/Ru0001-Chains

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Ru O H

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Cartesian

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H2O/Ru0001-Chains

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Ru O H

90 12 24

Cartesian

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H2O/Ru0001-Chains

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Ru O H

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Cartesian

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