Water adsorption and dissociation on Ni surface:

Effects of steps, promoters, coverage and self-aggregation

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Figure S1 Configuration of water dimer with a linear structure on Ni(111) surface.
Figure S2 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on Au/Ni_{1/9}(111) and Ag/Ni_{1/9}(111) surfaces. O-H distances (in Å) are labeled in each TS.
Figure S3 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on Au/Ni\textsubscript{1/4}(111) and Ag/Ni\textsubscript{1/4}(111) surfaces. O-H distances (in Å) are labeled in each TS.
Figure S4 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on Au/Ni$_{1/12}$(211) and Ag/Ni$_{1/12}$(211) surfaces. O-H distances (in Å) are labeled in each TS. Green balls show the position of the step. The letter “U/S/L” represents the location of “upper-terrace/step-edge/lower-terrace”.

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Figure S5 Structures of IS, TS and FS for water monomer (a) and dimer (b) dissociation on Ag/Ni_{1/6}(211) surface. O-H distances (in Å) are labeled in each TS. Green balls show the position of the step. The letter “U/S/L” represents the location of “upper-terrace/step-edge/lower-terrace”.

(a) \[ \text{H}_2\text{O} \xrightarrow{\text{Ag/Ni}_{1/6}(211)} \text{H} + \text{OH} \]

(b) \[ 2\text{H}_2\text{O} \xrightarrow{\text{Ag/Ni}_{1/6}(211)} \text{H} + \text{OH} + \text{H}_2\text{O} \]
Figure S6 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on Ag/Ni$_{1/12}$(211) and 2Ag/Ni$_{1/12}$(211) surfaces. O-H distances (in Å) are labeled in each TS. Green balls show the position of the step.