Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Water adsorption and dissociation on Ni surface: Effects of steps, promoters, coverage and self-aggregation

Yucheng Huang[*]*, Chongyi Ling, Meng Jin, Jinyan Du, Tao Zhou, Sufang Wang*

College of Chemistry and Material Science, Anhui Normal University, Wuhu, 241000, Peoples' Republic of China

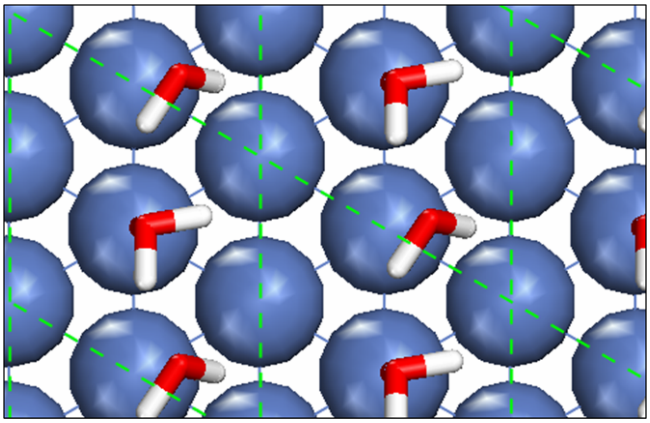

Figure S1 Configuration of water dimer with a linear structure on Ni(111) surface.

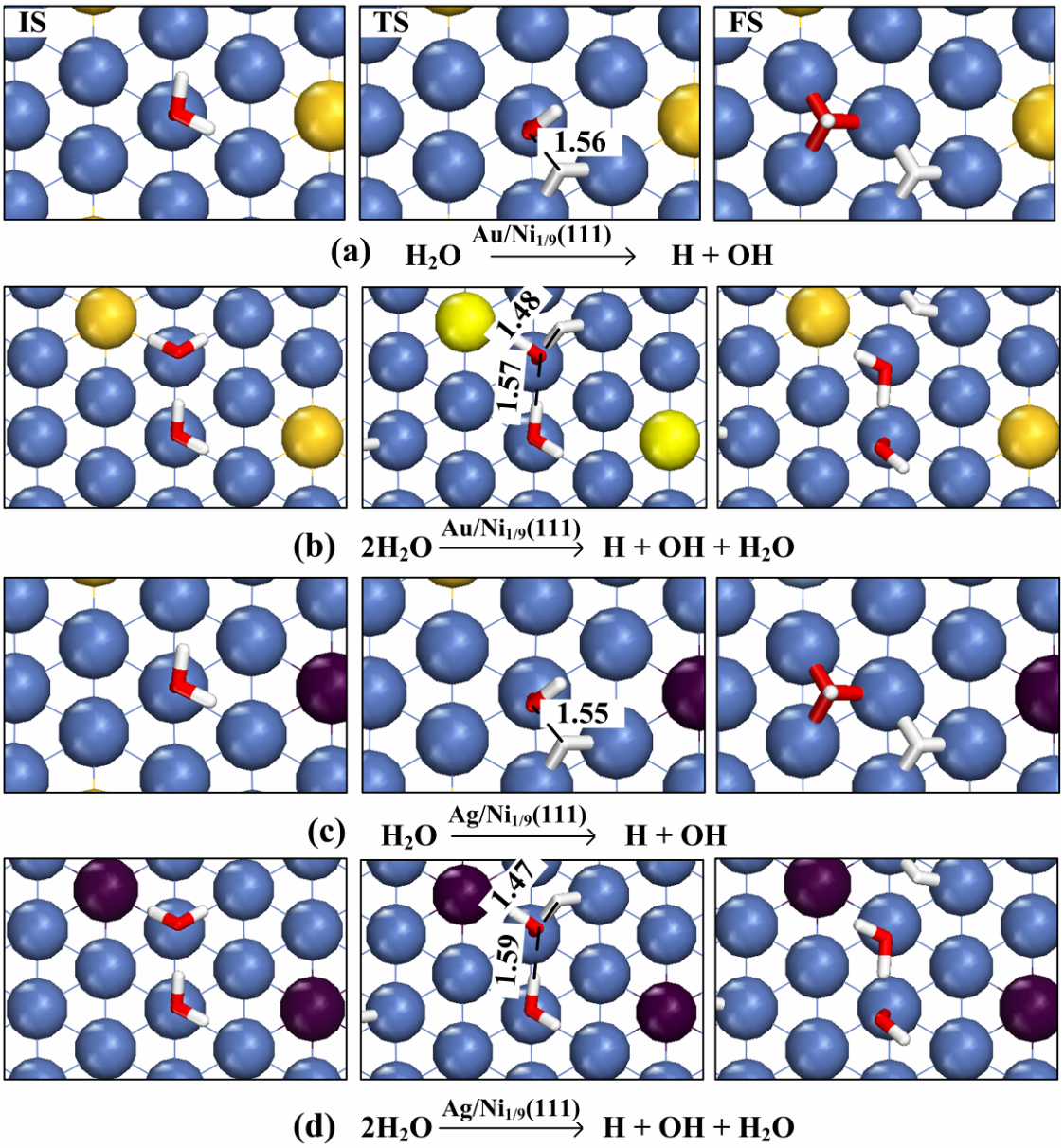

Figure S2 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on $Au/Ni_{1/9}(111)$ and $Ag/Ni_{1/9}(111)$ surfaces. O-H distances (in Å) are labeled in each TS.

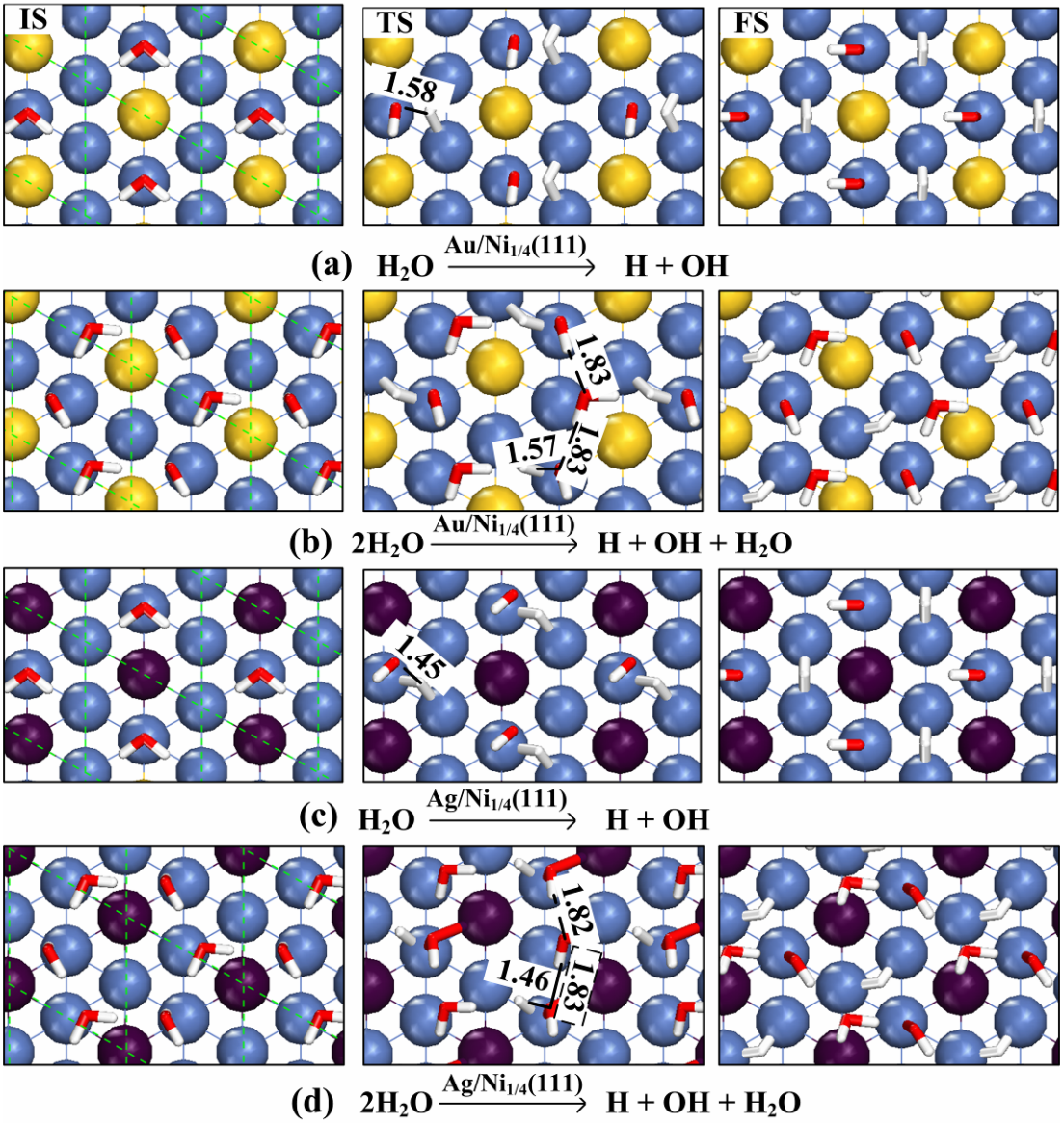

Figure S3 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on $Au/Ni_{1/4}(111)$ and $Ag/Ni_{1/4}(111)$ surfaces. O-H distances (in Å) are labeled in each TS.

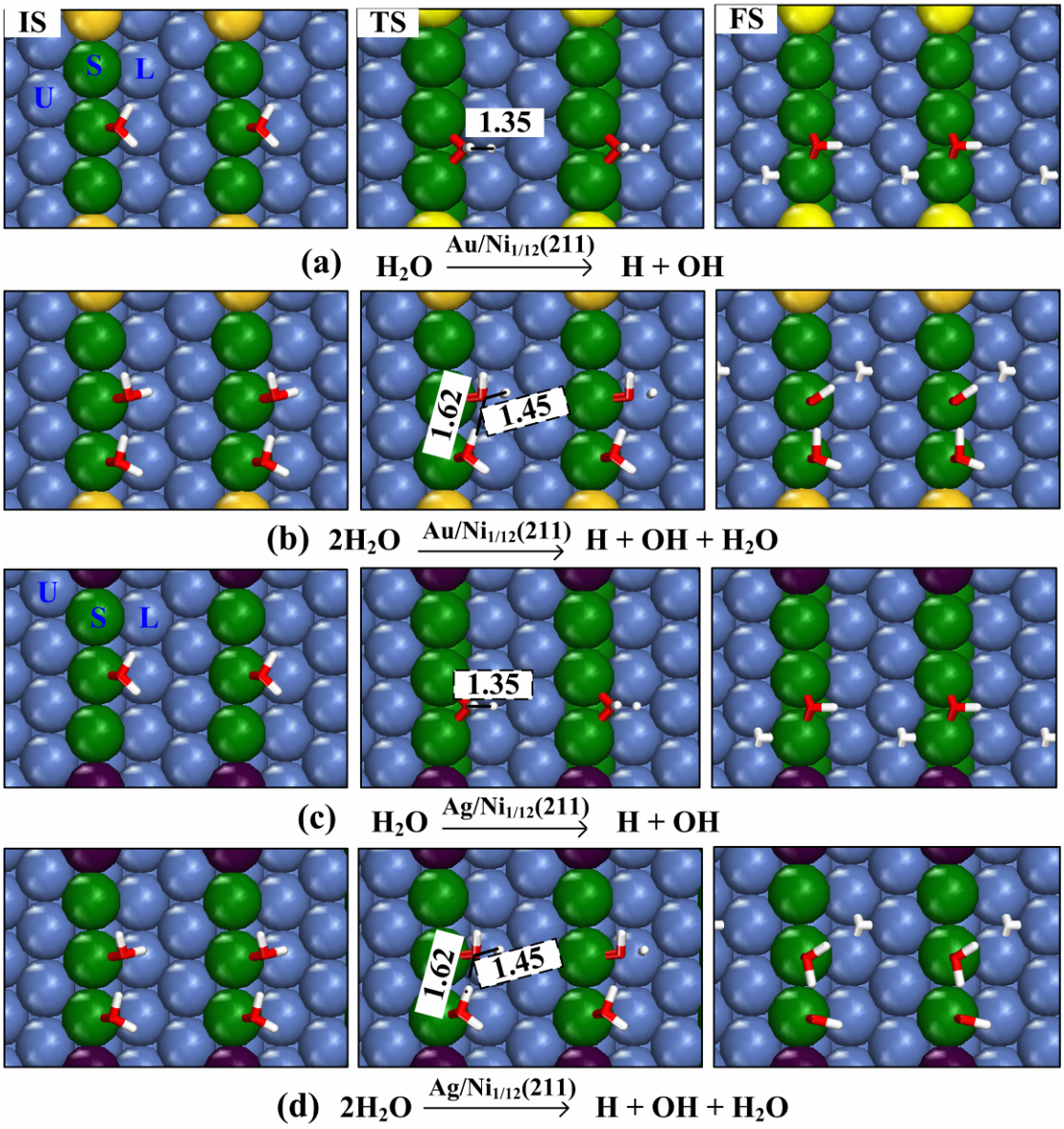

Figure S4 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on $Au/Ni_{1/12}(211)$ and $Ag/Ni_{1/12}(211)$ surfaces. O-H distances (in Å) are labeled in each TS. Green balls show the position of the step. The letter "U/S/L" represents the location of "upper-terrace/step-edge/lower-terrace".

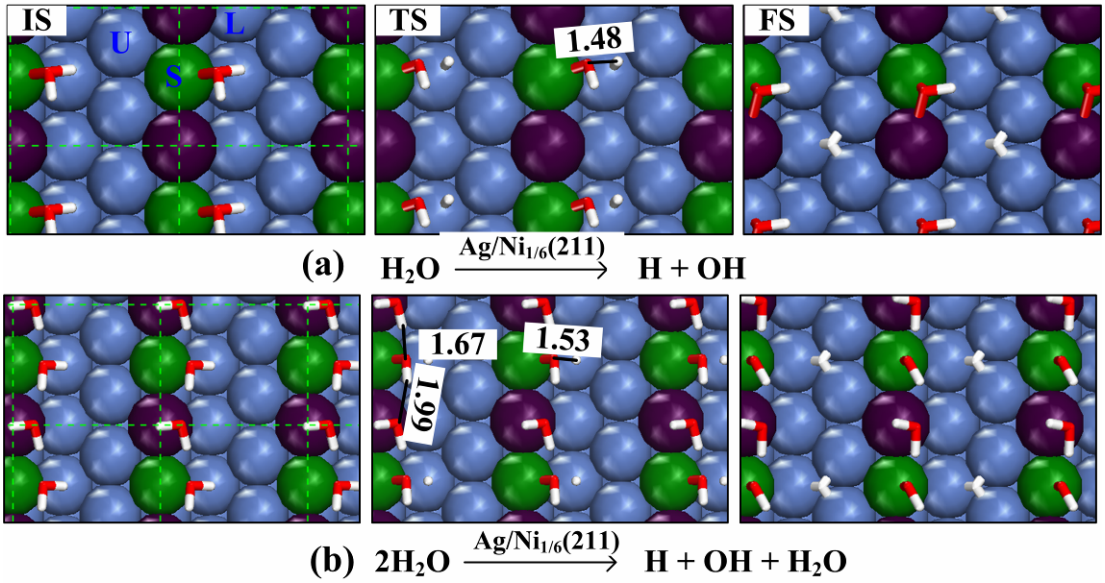

Figure S5 Structures of IS, TS and FS for water monomer (a) and dimer (b) dissociation on $Ag/Ni_{1/6}(211)$ surface. O-H distances (in Å) are labeled in each TS. Green balls show the position of the step. The letter "U/S/L" represents the location of "upper-terrace/step-edge/lower-terrace".

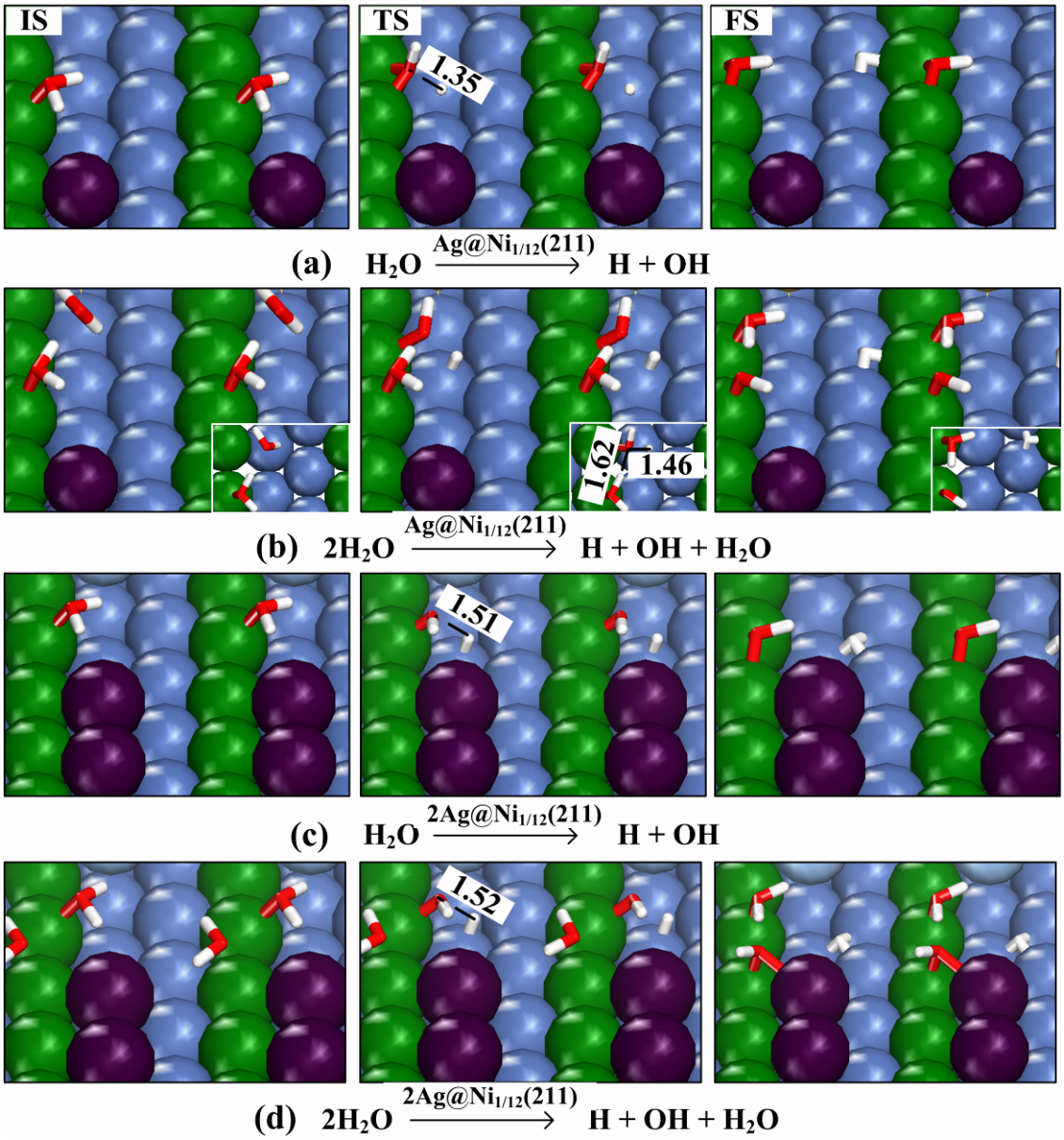

Figure S6 Structures of IS, TS and FS for water monomer (a, c) and dimer (b, d) dissociation on $Ag/Ni_{1/12}(211)$ and $2Ag/Ni_{1/12}(211)$ surfaces. O-H distances (in Å) are labeled in each TS. Green balls show the position of the step.