First-Principles study of water dissociation on PdZn near surface alloys

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Table S1. The reaction heat and energy barrier for water dissociation on 221^{Pd} step of PdZn(221) surface. Zero-point correction values are in parentheses.

	multilayer		monolayer	
	ΔH	E_a	ΔH	E_a
monomer	0.62 (0.48)	1.14 (0.95)	0.28 (0.16)	0.95(0.72)
1D-chain	0.62 (0.44)	1.14 (0.95)	0.31 (0.14)	0.90 (0.73)

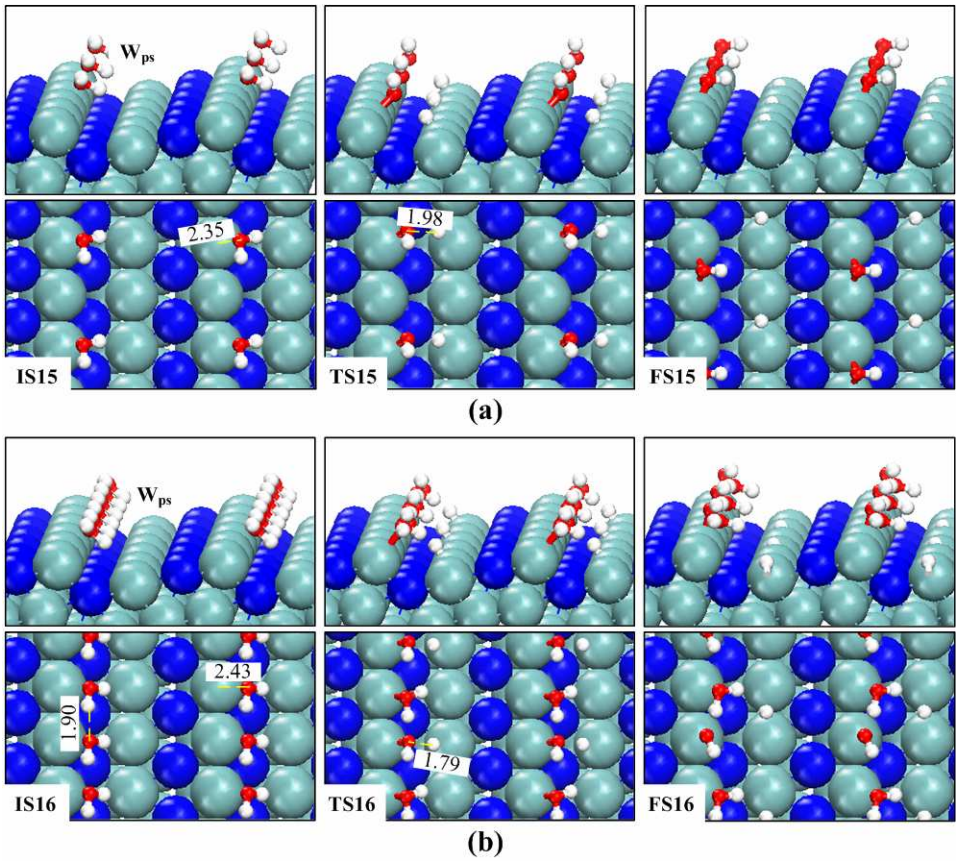

Figure S1. Structures of initial states, transition states and final states for water monomer (a) and 1D-chain (b) dissociation on 221^{Pd} surface of PdZn multilayer. The upper/lower panel is the

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side/top view. Blue balls denote Zn atoms. The O-Zn and O-H bond length are in Å.

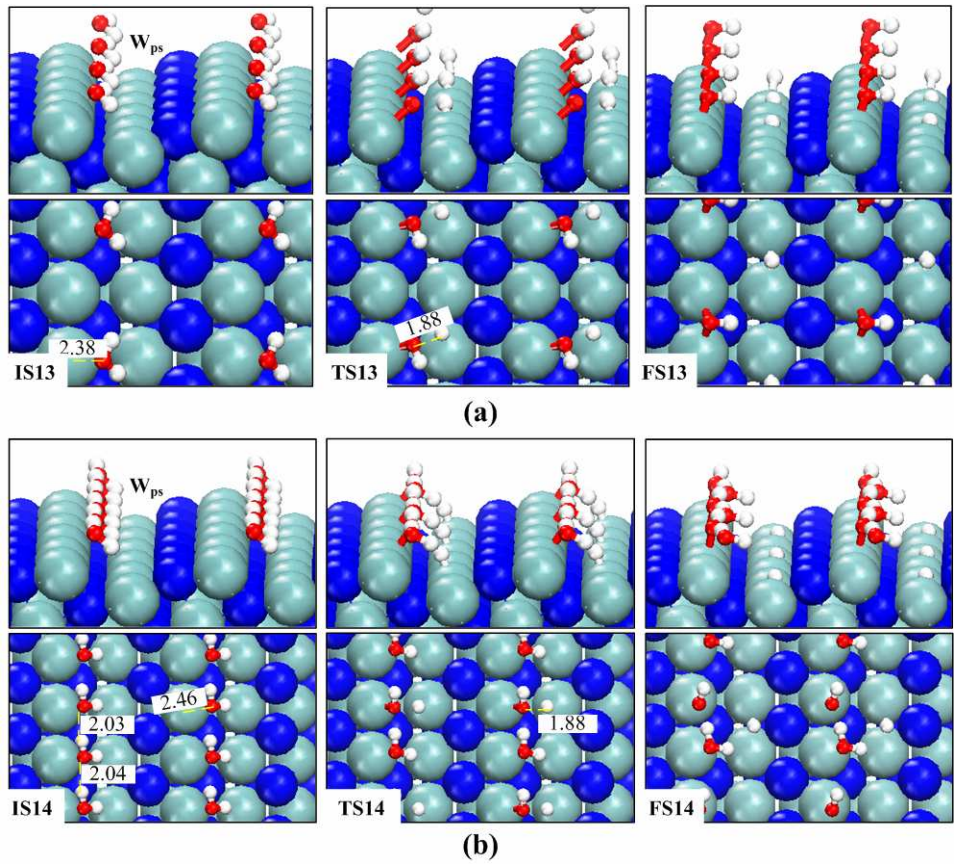

Figure S2. Structures of initial states, transition states and final states for water monomer (a) and 1D-chain (b) dissociation on 221^{Pd} surface of PdZn monolayer. The upper/lower panel is the side/top view. Blue balls denote Zn atoms. The O-Zn and O-H bond length are in Å.