Surface Charge Effects on the Thermodynamics and Kinetics of Hydrogen Evolution Reaction on Pt(111) Using a Modified Grand-Canonical Potential Kinetics Method

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Table S1. Corrections from zero-point energy (ΔZPE) and charge extrapolation (ΔCE) for canonical barriers and reaction energies.

		$\Delta E^{\ddagger}$ (eV)	ΔZPE (eV)	ΔCE (eV)	$\Delta G^{\ddagger}$ (eV)
Tafel	reaction barrier	0.79	-0.11	-0.02	0.66
	reaction energy	0.14	-0.02	0.03	0.16

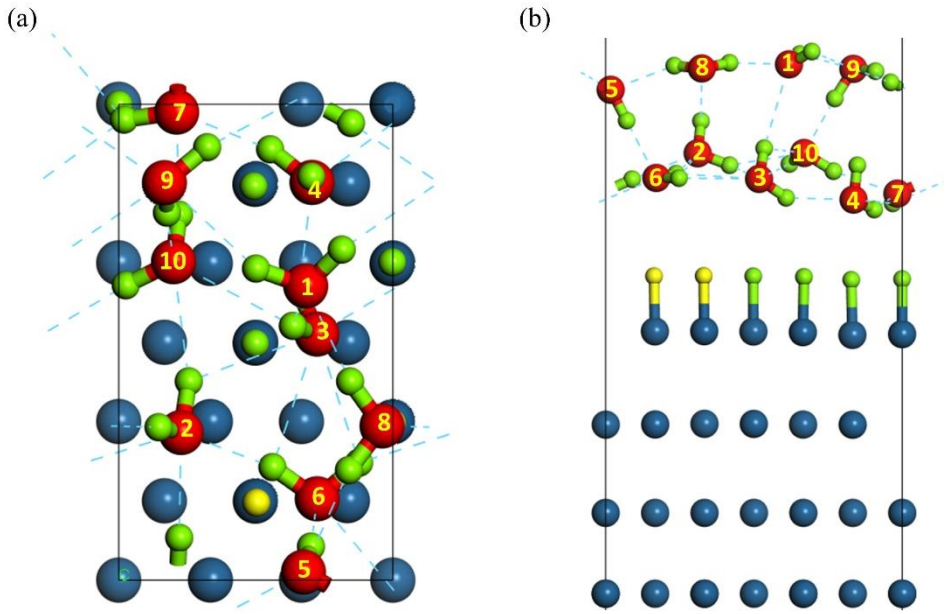

Figure S1. Structural models of Pt (111)/H_2O (a) Top and (b) side views of the grand-canonical initial state structure of the Tafel reaction in acid. There are 10 H_2O molecules marked with numerals in the water layer.