Water Chemistry on Two-Dimensional Silicates Studied by Density Functional Theory and Temperature-Programmed Desorption

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Highlights

- Water adsorbs weakly on 2D SiO_2 but silanol groups increase the adsorption strength three-fold and Al substitution five-fold.
- Water can permeate 2D SiO_2 to reach a Pd(111) support where adsorption and dissociation is largely unaffected by the SiO_2 overlayer.
- Chemical bonds between 2D aluminosilicates and the metal support inhibit water dissociation and protonation of the aluminosilicate at the metal interface.
- Removing charge balancing protons from 2D aluminosilicate surfaces proceeds through a dehydration pathway that requires temperatures >1100 K, irrespective of the presence of a metal substrate.
- Experiments confirm that Al incorporation increases water adsorption strength and provide no evidence of loss of Brønsted acid sites up to 800 K.