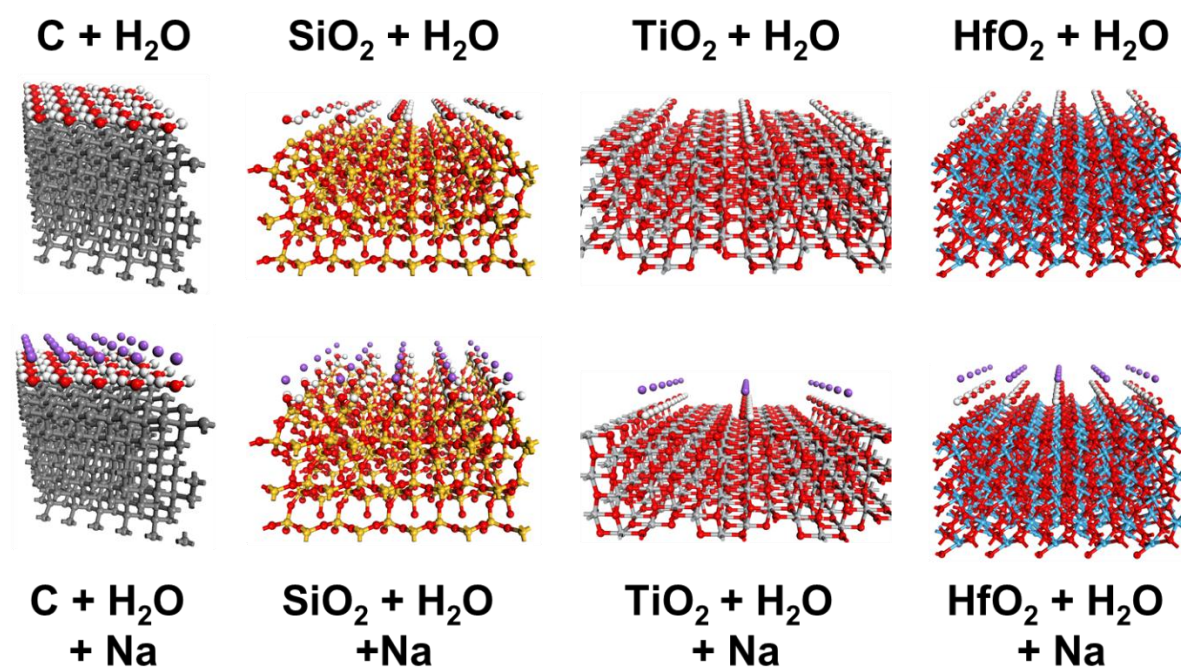


Supplementary Information

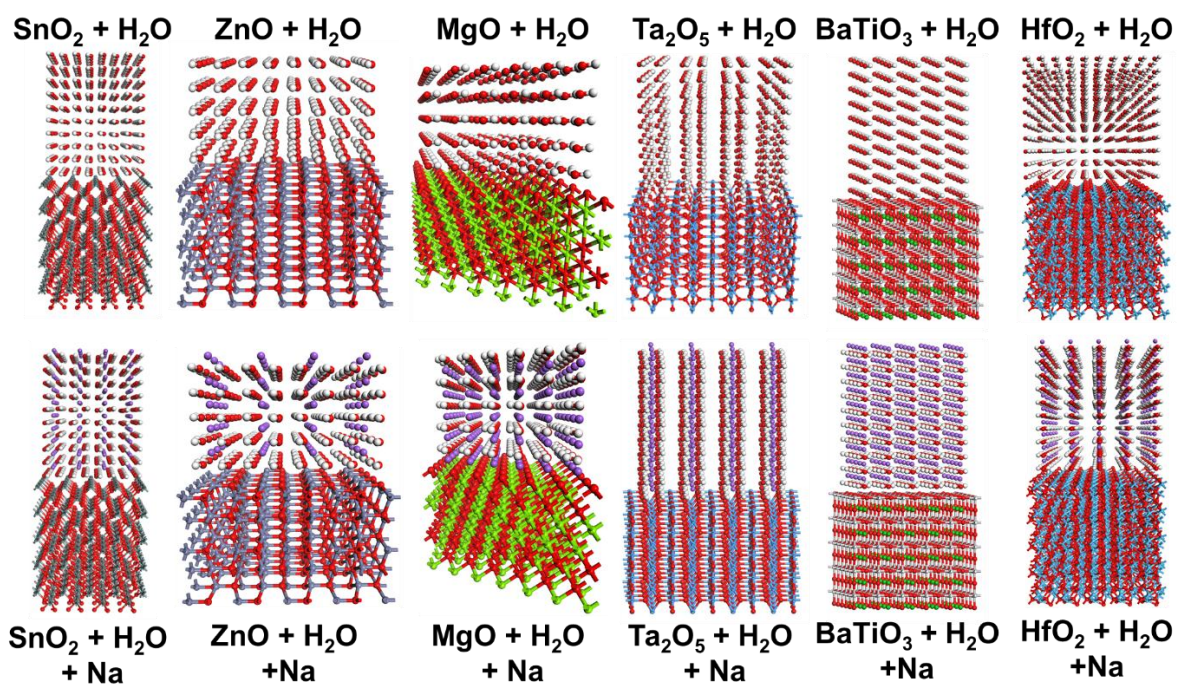
Understanding Contact Electrification at Liquid-Solid Interfaces from Surface Electronic Structure

Sun et al.

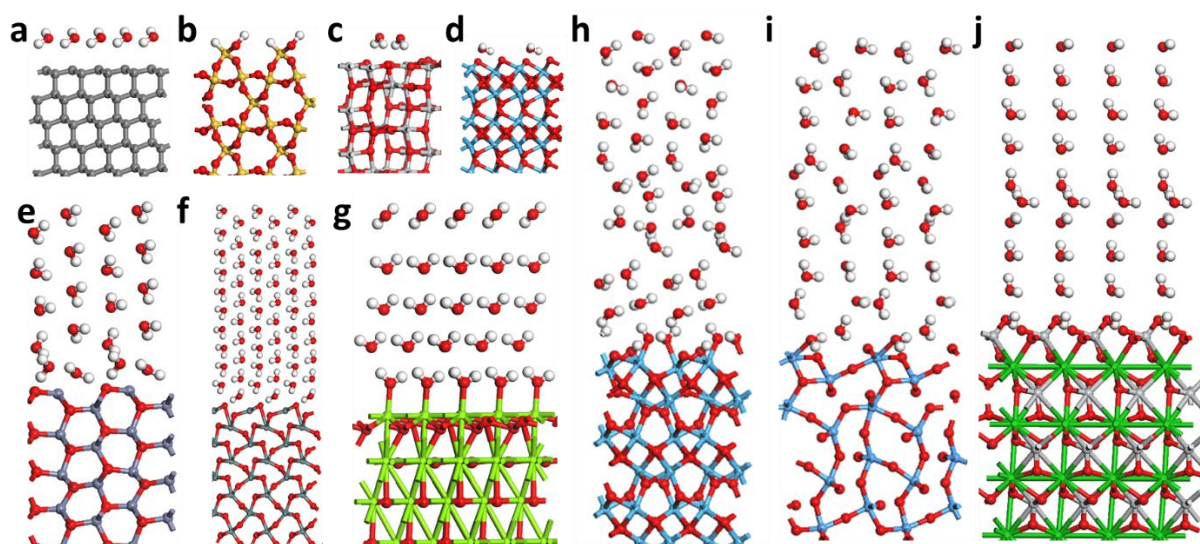
Supplementary Figures



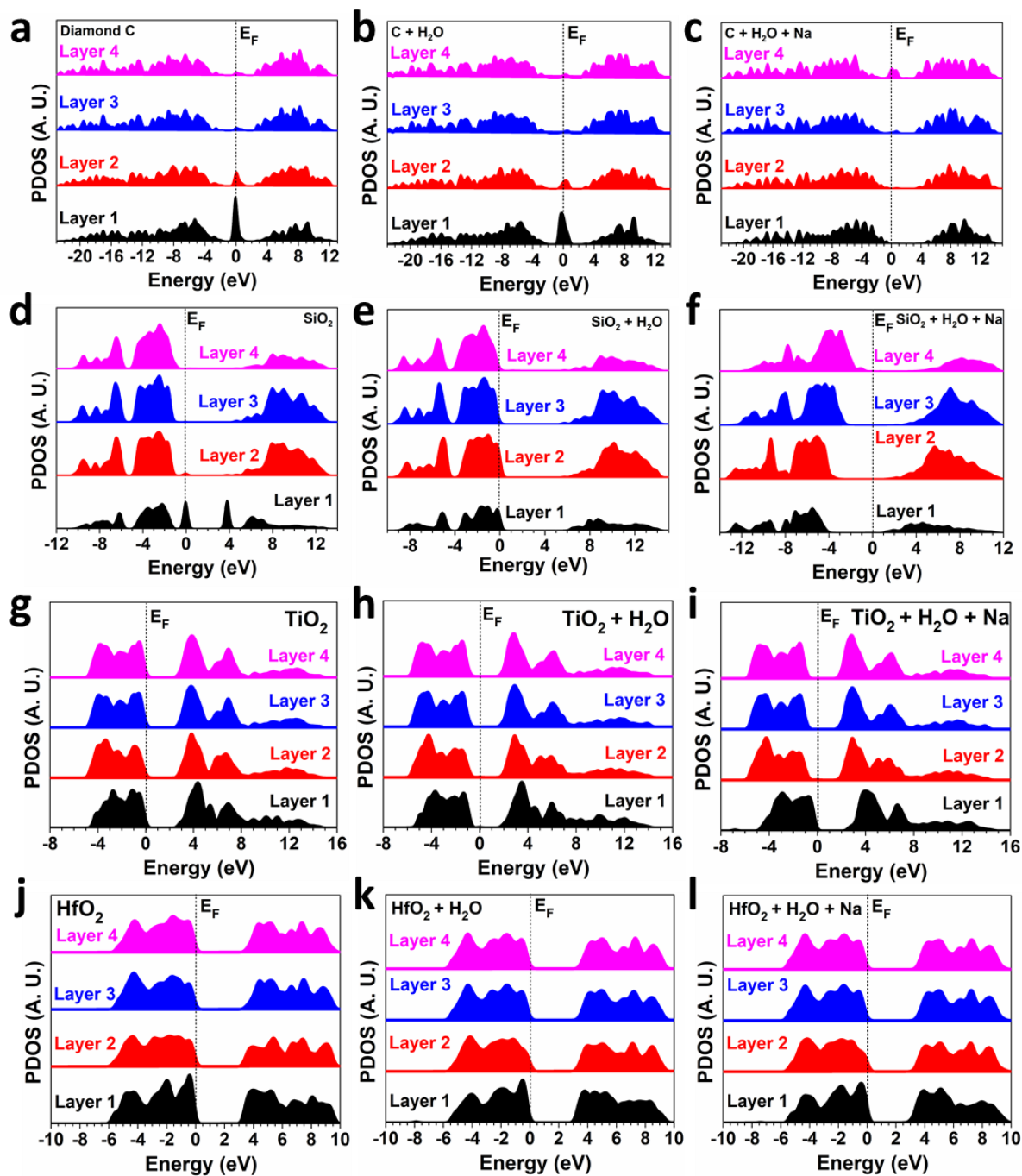
Supplementary Fig. 1 The simulation models for multi-layered water and solution in insulator diamond, dielectric insulator SiO₂, transition metal oxide TiO₂ and high-K oxide HfO₂.



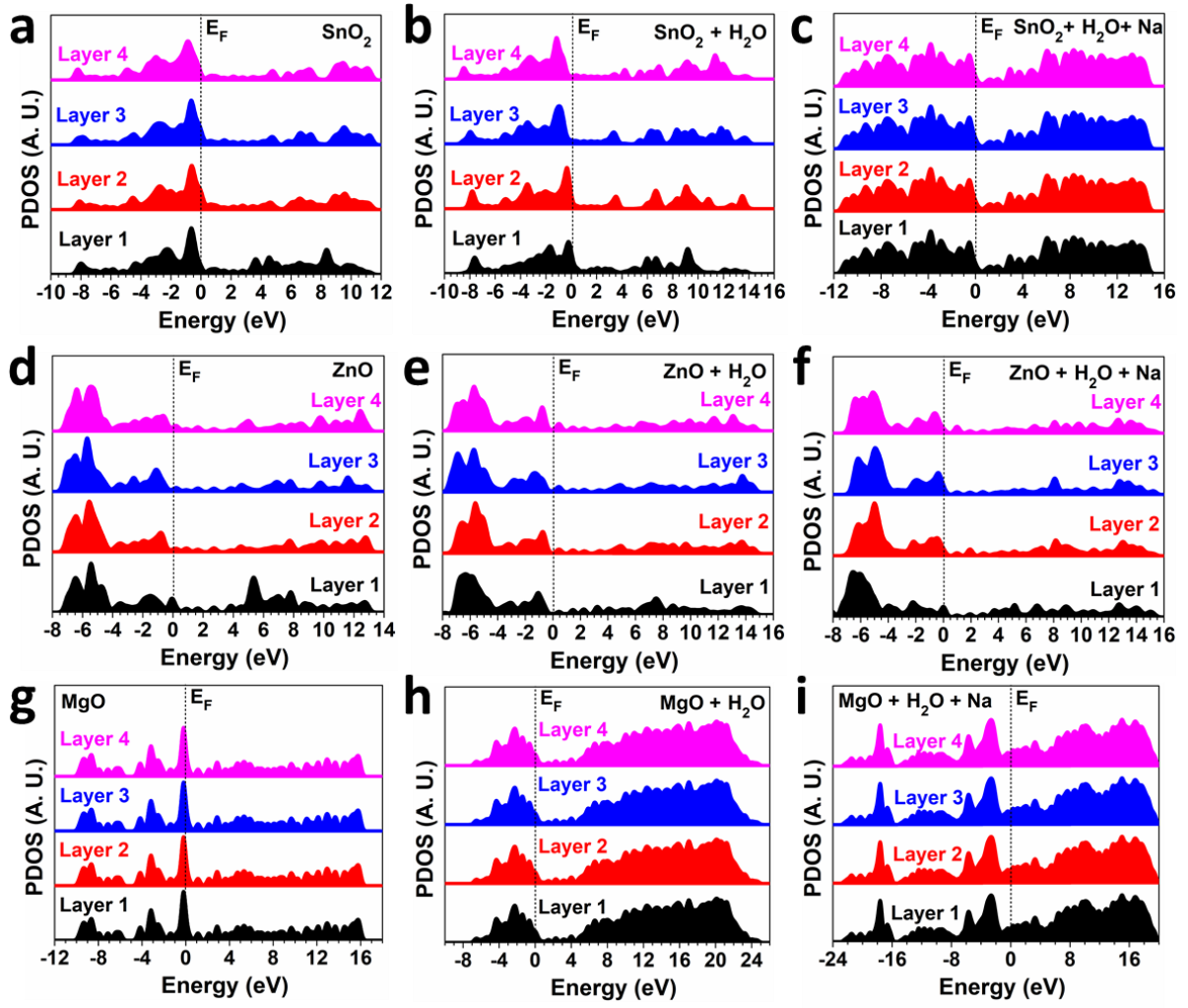
Supplementary Fig. 2 The simulation models for multi-layered water and solution in SnO₂, ZnO, MgO, Ta₂O₅ and HfO₂.



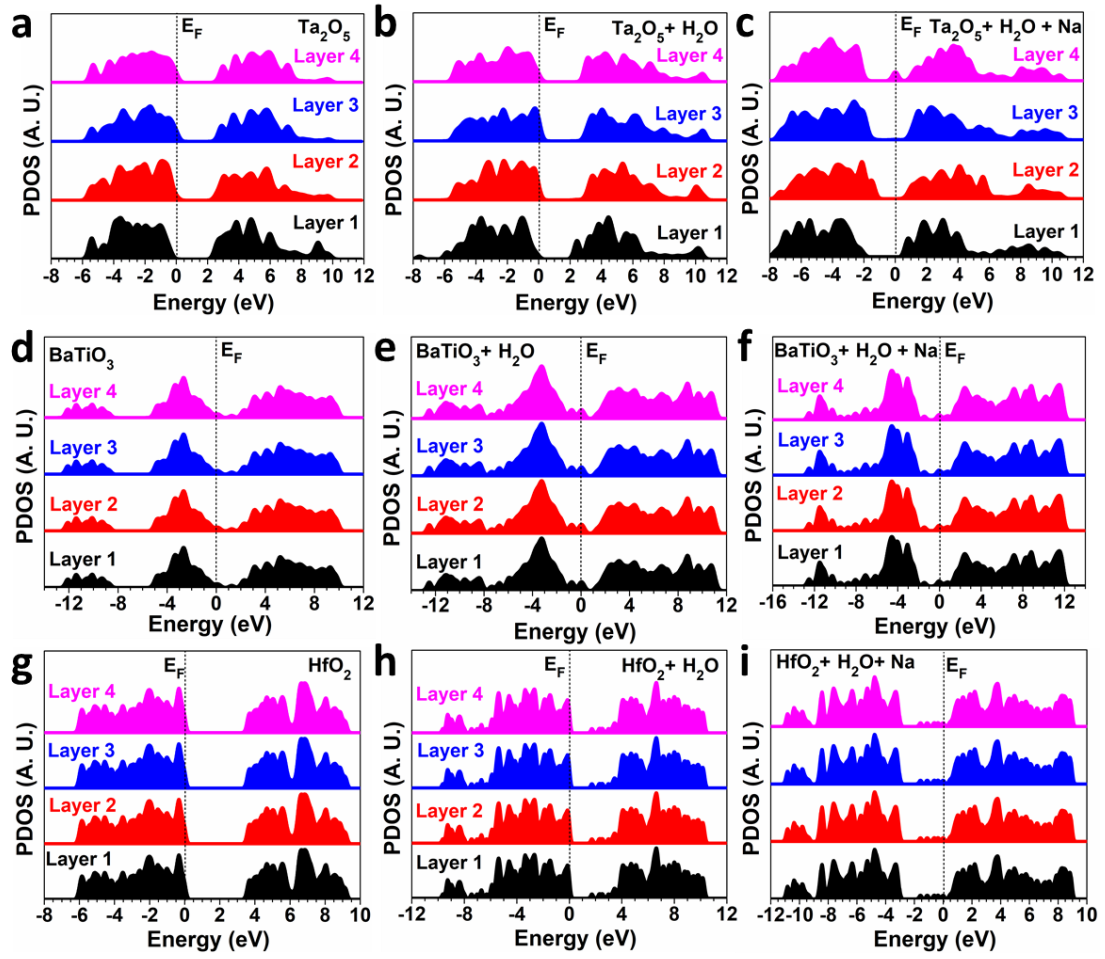
Supplementary Fig. 3 The side view of different solids after contacting with water molecules. Single-layered water on (a) Diamond; (b) SiO₂, (c) TiO₂, and (d) HfO₂. Multi-layered water on (e) ZnO; (f) SnO₂, (g) MgO, (h) HfO₂, (i) Ta₂O₅ and (j) BaTiO₃.



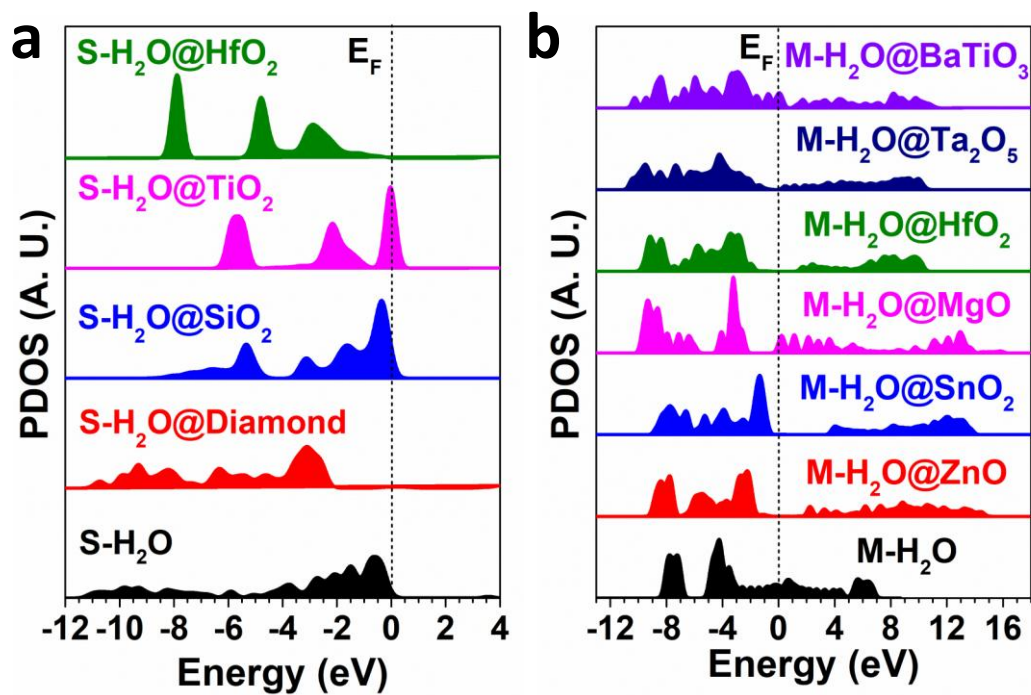
Supplementary Fig. 4 The layer-dependent TDOS of each solid after contacting with single-layered water. (a) diamond C, (b) C + H₂O and (c) C + H₂O + Na. (d) SiO₂, (e) SiO₂ + H₂O and (f) SiO₂ + H₂O + Na. (g) TiO₂, (h) TiO₂ + H₂O and (i) TiO₂ + H₂O + Na. (j) HfO₂, (k) HfO₂ + H₂O and (l) HfO₂ + H₂O + Na.



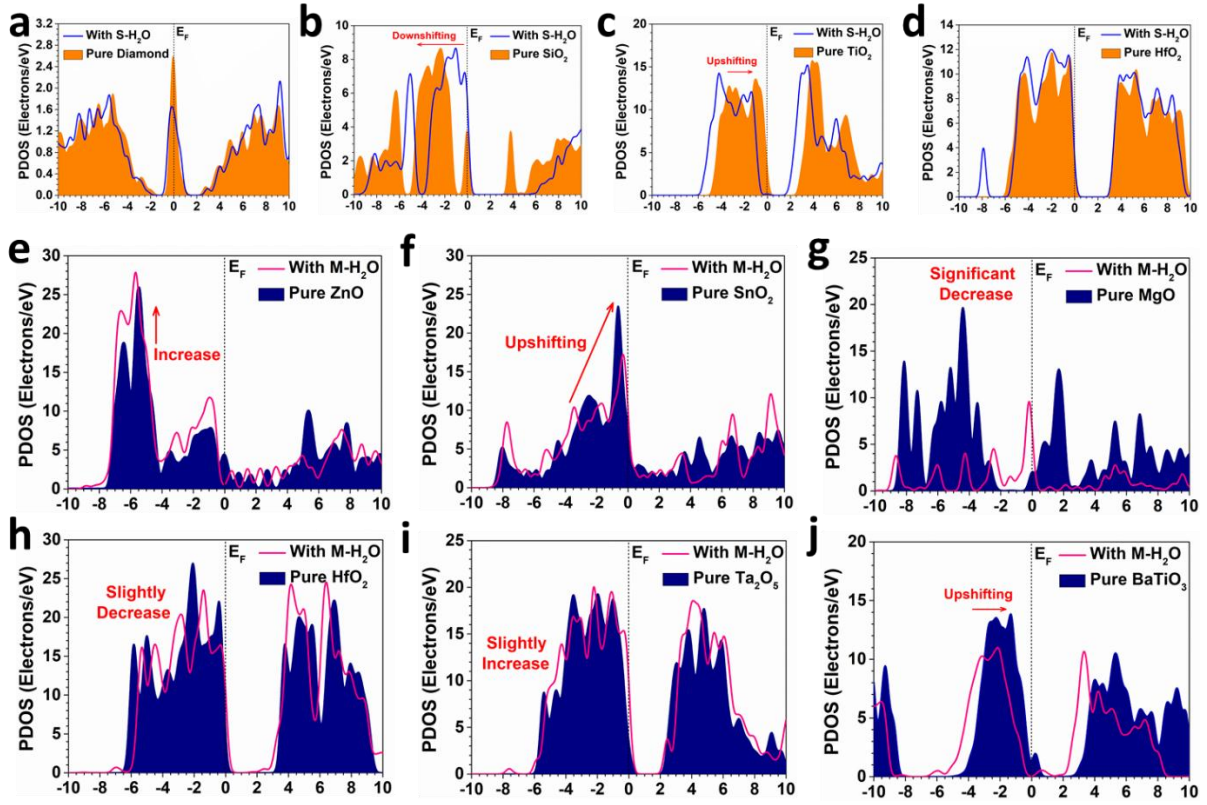
Supplementary Fig. 5 The layer-dependent TDOS of each solid after contacting with multi-layered water. (a) SnO_2 , (b) $\text{SnO}_2 + \text{H}_2\text{O}$ and (c) $\text{SnO}_2 + \text{H}_2\text{O} + \text{Na}$. (d) ZnO , (e) $\text{ZnO} + \text{H}_2\text{O}$ and (f) $\text{ZnO} + \text{H}_2\text{O} + \text{Na}$. (g) MgO , (h) $\text{MgO} + \text{H}_2\text{O}$ and (i) $\text{MgO} + \text{H}_2\text{O} + \text{Na}$.



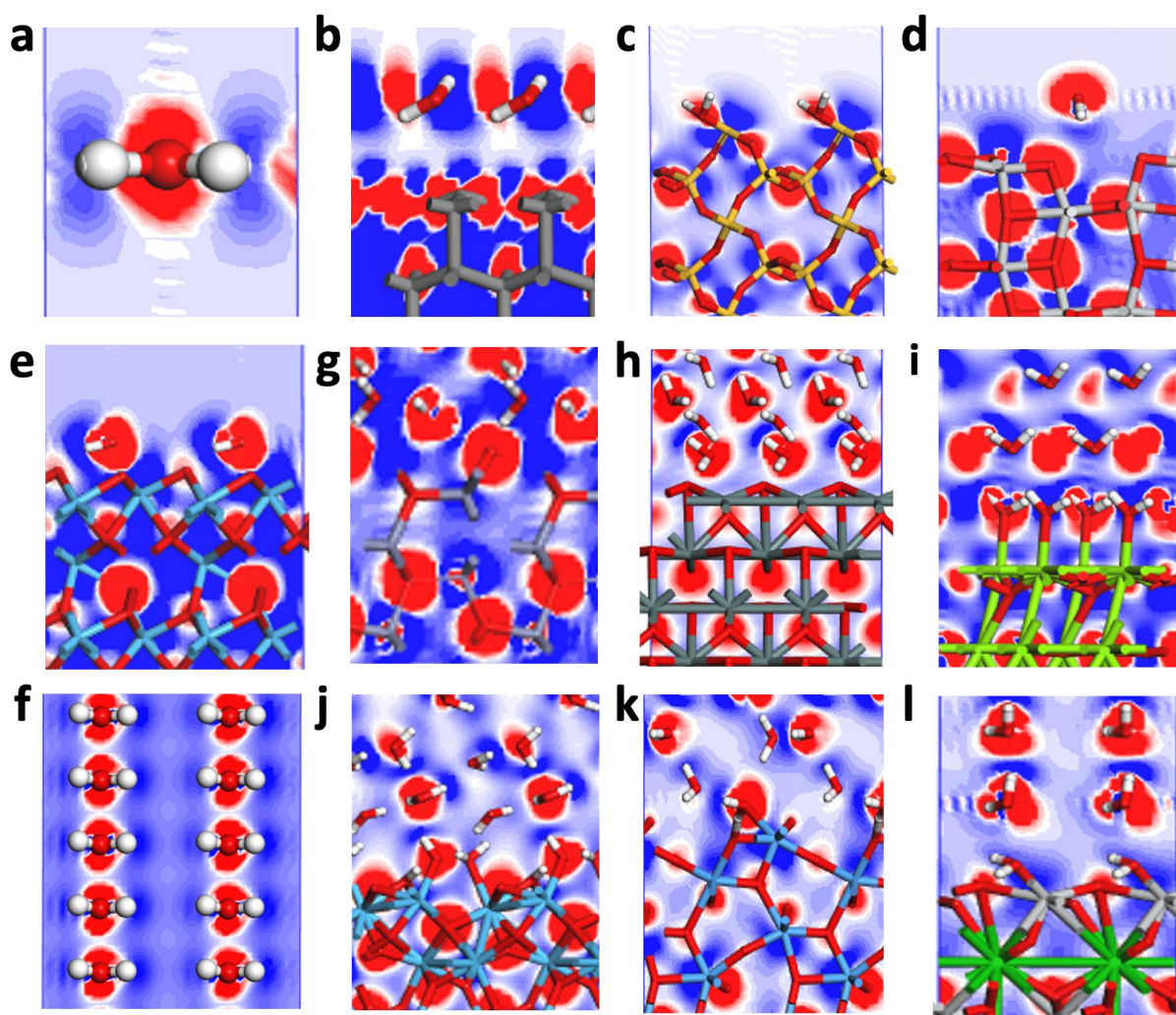
Supplementary Fig. 6 The layer-dependent TDOS of each solid after contacting with multi-layered water. (a) Ta_2O_5 , (b) $\text{Ta}_2\text{O}_5 + \text{H}_2\text{O}$ and (c) $\text{Ta}_2\text{O}_5 + \text{H}_2\text{O} + \text{Na}$. (d) BaTiO_3 , (e) $\text{BaTiO}_3 + \text{H}_2\text{O}$ and (f) $\text{BaTiO}_3 + \text{H}_2\text{O} + \text{Na}$. (g) HfO_2 , (h) $\text{HfO}_2 + \text{H}_2\text{O}$ and (i) $\text{HfO}_2 + \text{H}_2\text{O} + \text{Na}$.



Supplementary Fig. 7 Electronic structure comparisons of water on different solid surfaces. (a) The single-layered water on different solid surfaces. (b) The multi-layered water on different solid surfaces.



Supplementary Fig. 8 Electronic comparison of the top two-layers in the solids after contacting electrification with water. Single-layered water on (a) Diamond; (b) SiO₂, (c) TiO₂, and (d) HfO₂. Multi-layered water on (e) ZnO; (f) SnO₂, (g) MgO, (h) HfO₂, (i) Ta₂O₅ and (j) BaTiO₃.



Supplementary Fig. 9 Electronic density difference of the water-solid interface after contact electrification with water. (a) Single-layered water. Single-layered water on (b) Diamond; (c) SiO_2 , (d) TiO_2 , and (e) HfO_2 . (f) Multi-layered water. Multi-layered water on (g) ZnO ; (h) SnO_2 , (i) MgO , (j) HfO_2 , (k) Ta_2O_5 and (l) BaTiO_3 .

Supplementary Table

Supplementary Table S1. The summarized data for electronic parameters and charge transfer in different liquid/oxide systems

Solid	$\Delta E_{ads}(\text{eV})$	ϕ_{Work} Function (eV)	$\Delta\phi_{\text{Work}}$ Function (eV)	Charge Q (nC)	Dielectric Constant	P (pinning factor)
SiO ₂	-2.48	6.46	0.185	1.44	2.49	0.82
TiO ₂	0.02	6.11	-0.12	0.02	10.2	0.11
HfO ₂	-1.52	5.33	-1.24	0.56	5.45	0.34
ZnO	3.10	5.03	-0.02	14.5	11.3	0.09
Ta ₂ O ₅	-1.64	3.58	-2.76	0.06	4.87	0.40
MgO	11.11	4.83	0.25	9.23	6.77	0.23
SnO ₂	13.54	6.16	-0.07	20.8	8.42	0.15