Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Implications of the Fractional Charge of Hydroxide at the Electrochemical Interface

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Note 1

We now show that the previous charge overlap analysis for hydronium [1] does not extend to the case of hydroxide. Figure S1 shows the charge overlap analysis in the case of a hydronium and hydroxide ion in panels (a) and (b) respectively. To simulate the charge density of the slab and solvent in isolation, continuum solvation and an excess surface charge via VASPsol was used on the two systems separately.

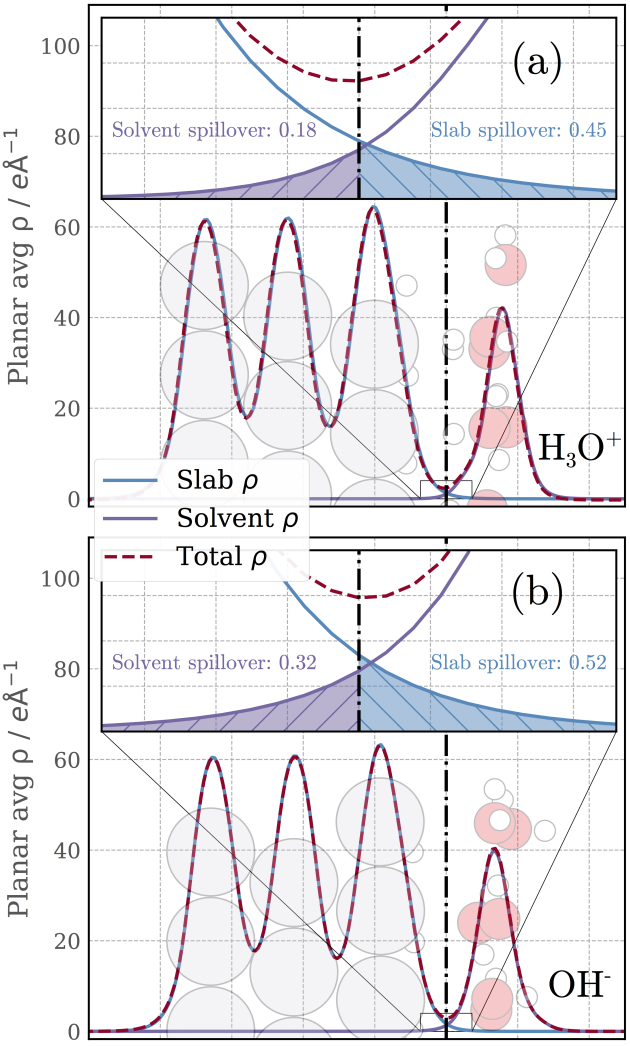

Figure S1: Charge density overlap analysis for the case of (a) hydronium and (b) hydroxide. In the case of hydronium, the slab, with an excess charge of $-1.0\ e$, spills 0.45 electrons into the electrolyte region, while the electrolyte, with an excess charge of $1.0\ e$, only spills 0.18 electrons into the slab region. This results in a net charge of $1.0 - (0.45 - 0.18) = 0.73\ e$ on the hydronium ion, in close agreement with Bader charge partitioning. However, in the case of hydroxide, a similar analysis predicts an ion charge of $-1.2\ e$, in contrast to the predicted $-0.8\ e$ from Bader.

While the charge overlap analysis for hydronium agrees quite well with the predicted ionic charge from Bader analysis, as outlined in our previous work,[1] the same analysis does not extend to the case of hydroxide. Figure S1(a) shows that in the case of hydronium, the slab electron density spilling into the electrolyte region results in a loss of 0.45 e, while the solvent density in the slab region results in a gain of 0.18 e, for a total net charge of $1.0 - (0.45 - 0.18) = 0.73\,e$ on the hydronium ion. At the GGA level, Bader predicts an ionic charge of 0.73 e, and at the hybrid level 0.77 e, within the previously stated error margin of 0.05 e. However, a similar argument in the case of hydroxide (panel (b) of Figure S1) shows that the predicted ionic charge of hydroxide from charge overlap is -1.2 e, while Bader predicts -0.8 e. We hypothesize that this is due to the closer proximity of the outer Helmholtz plane to the surface in the case of hydroxide. Even when the surface is fully covered by hydrogen, the solvent bilayer interacts strongly with the surface, with one water molecule arguably physisorbed to the surface, which affects the extracted charge. The slab density then has a larger spillover region into the solvent, despite having a more positive surface charge in the case of hydroxide. The close proximity combined with the ambiguously defined cutoff between the electrolyte and slab regions therefore make the charge overlap analysis less reliable in the case of hydroxide. In such a case, the densities of the slab and solvent cannot simply be added separately to obtain an accurate ionic charge. Nonetheless, we note that because the charge of hydroxide quickly approaches -1.0 e at both the GGA and hybrid levels as the ion is moved away from the surface, the non-unity charge observed in the outer Helmholtz plane is not due to DFT self-interaction errors.

Note 2

In Figure S2, we show the projected densities of states of the hydroxide containing water bilayer near a platinum surface. The electrolyte LUMO states are clearly visible above the Fermi level.

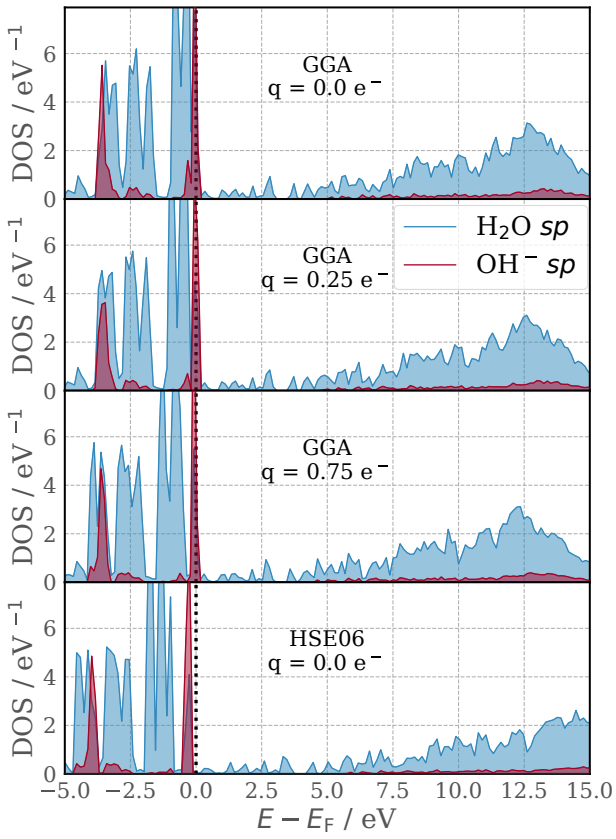

Figure S2: Expanded view of projected densities of states for a water bilayer containing one hydroxide ion near the interface.

Note 3

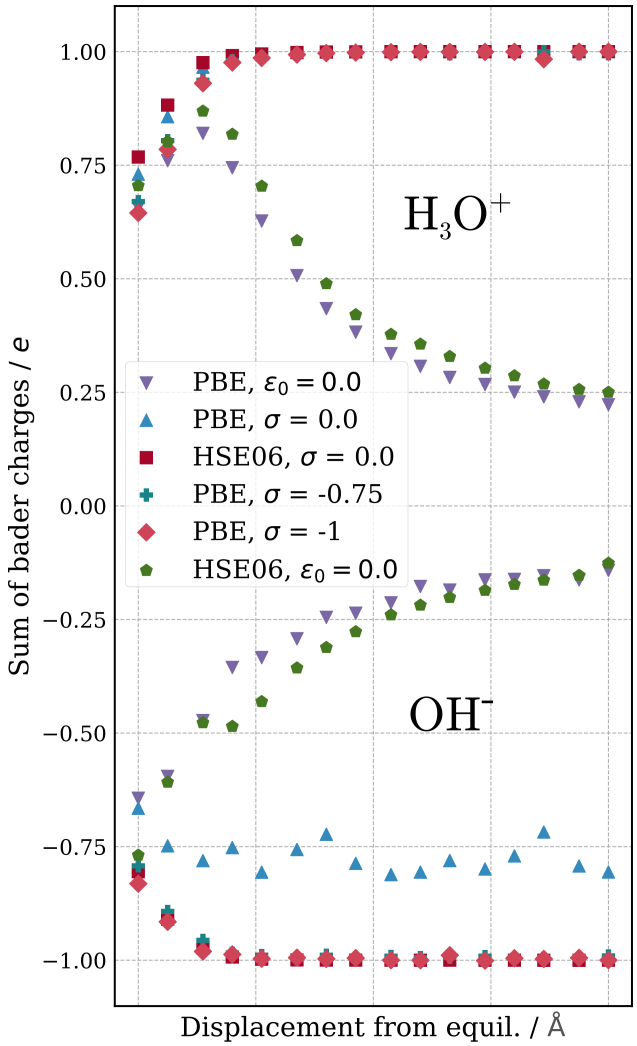

Figure S3: Expanded charging plot illustrating the decay of hydroxide and hydronium charge far from the surface without the dielectric continuum present to stabilize the ion, as found in Ref. 2 by Andreussi et al.

Note 4

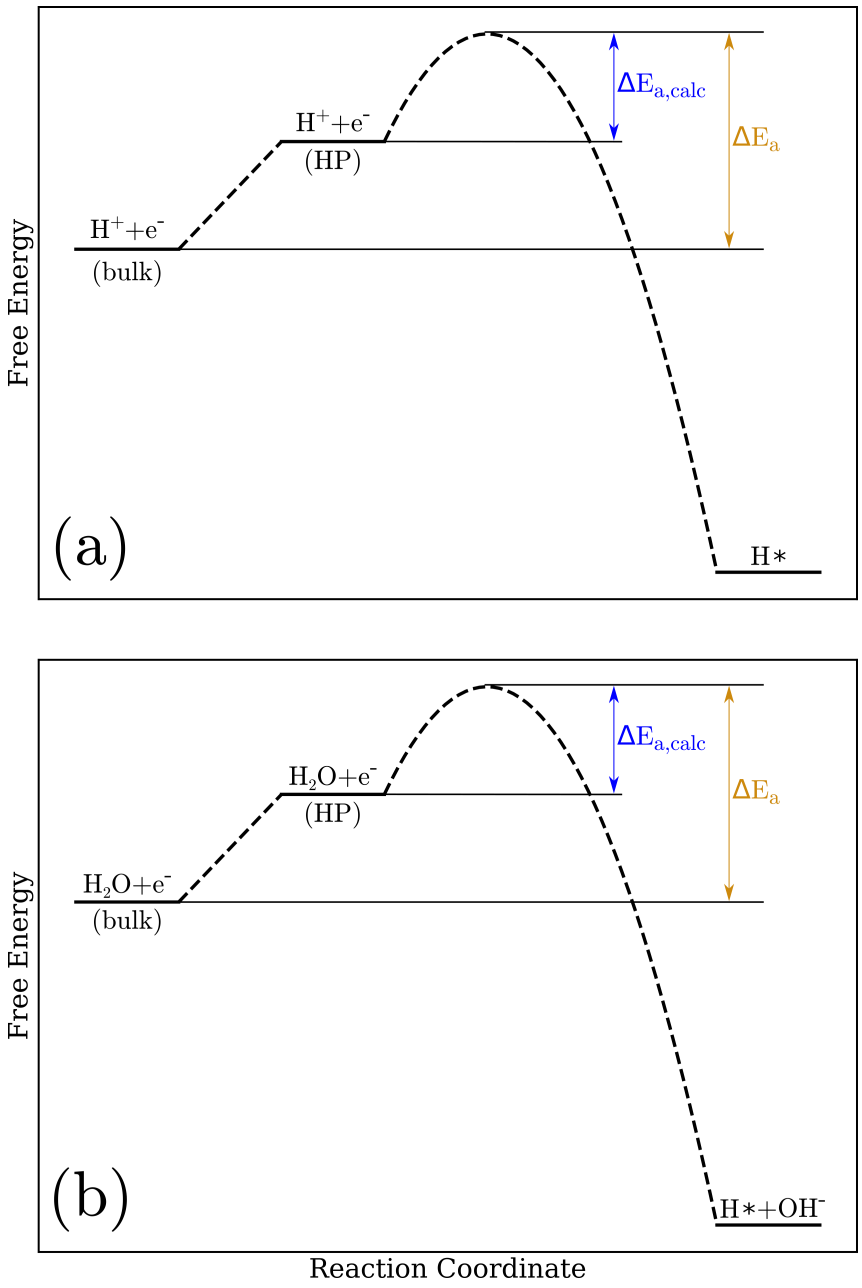

Figure S4: Illustration of appropriate referencing in the calculation of electrochemical barriers for (a) the case of hydronium, and (b) the case of hydroxide. The electrochemical reaction barrier as measured from the calculation's initial state is shown in blue as $\Delta E_{\mathrm{a,calc}}$ while the appropriately references electrochemical reaction barrier is shown in orange as ΔE_{a}. The lack of equilibrium between the initial state of the calculation (with the ion in the Helmholtz Plane (HP)), and the true initial state (with the ion in the bulk, far from the surface) is shown by the difference in free energy between the two states.

References

(1) Chen, L. D.; Bajdich, M.; Martirez, J. M. P.; Krauter, C. M.; Gauthier, J. A.; Carter, E. A.; Luntz, A. C.; Chan, K.; Nørskov, J. K. Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. *Nature Communications* **2018**, *9*, 3202.

(2) Nattino, F.; Dupont, C.; Marzari, N.; Andreussi, O. Functional extrapolations to tame unbound anions in density-functional theory calculations. *arXiv preprint arXiv:1906.00822* **2019**,

Tables and data: figures from the main text

Figure 1

Panel (a)

POSCAR file for both GGA and hybrid level calculations:

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     4.2089965459999998    7.2901958670000004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.4216483592290956
   H    O    Pt
    22     6    27
Selective dynamics
Direct
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  0.3423035848940543  0.0065042506900141  0.5509552268554145   T   T   T
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0.0763150497558556	0.5928643494176100	0.5881192872591541	T	T	T
0.0013111189316533	0.8995494961923214	0.5905074345835928	T	T	T
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0.9526241014601169	0.7116234293668882	0.5485001128530982	T	T	T
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0.4468257974661256	0.1127625969627530	0.4302812586437952	T	T	T
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0.0327704680625232	0.9959974345377489	0.5983788128060468	T	T	T
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0.6423546507305673	0.6999982964060862	0.5992031363677626	T	T	T
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0.7777777077055603	0.7777774566615747	0.2465349645567372	F	F	F
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0.3319592496821784	0.6691492646844495	0.3987891902509375	T	T	T
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INCAR file for GGA calculation:

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 SIGMA = 0.050000
 EDIFF = 1.00e-04
 EDIFFG = -5.00e-02
 PREC = Accurate
 GGA = PE
 ALGO = Normal
 ISMEAR = 0
 NELM = 250
 IBRION = 2
 NSW = 0
 LORBIT = 11
 NCORE = 16
 LASPH = .TRUE.
 LVHAR = .TRUE.
 AMIX = 0.1
 BMIX = 0.01
 LSOL = .TRUE.
 TAU = 0.0
 LAMBDA_D_K = 3.0
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INCAR for hybrid calculation:

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INCAR created by Atomic Simulation Environment
 ENCUT = 400.000000
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EDIFFG = -5.00e-02

PREC = Accurate

GGA = PE

ISMEAR = 0

NELM = 100

IBRION = 2

NSW = 0

LORBIT = 11

NCORE = 16

LASPH = .TRUE.

LSOL = .TRUE.

TAU = 0.0

LAMBDA_D_K = 3.0


/*hybrid flags*/

ALGO = Damped

HFSCREEN = 0.2

TIME = 0.07

AEXX = 0.25

LHFCALC = .TRUE.
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Panel (b)

POSCAR file for both GGA and hybrid calculations:

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  1.00000000000000
```

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     4.2089970000000001    7.2901959999999999    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.8725200000000015
   H    Pt   O
    20    27     6
Selective dynamics
Direct
  0.9093717051139407  0.9872762843161524  0.5922504354448108   T   T   T
  0.0324690687467069  0.9945582454904098  0.6314611321631816   T   T   T
  0.3680717480403146  0.4472345353400584  0.5856424140564016   T   T   T
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INCAR file for GGA calculation:

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 EDIFFG = -5.00e-02
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 GGA = PE
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 ISMEAR = 0
 NELM = 250
 IBRION = 2
 NSW = 0
 LORBIT = 11
 NCORE = 16
 LASPH = .TRUE.
 LVHAR = .TRUE.
 AMIX = 0.1
 BMIX = 0.01
 LSOL = .TRUE.
```

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 TAU = 0.0
 LAMBDA_D_K = 3.0
```

INCAR file for hybrid calculation:

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 ISMEAR = 0
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 IBRION = 2
 NSW = 0
 LORBIT = 11
 NCORE = 16
 LASPH = .TRUE.
 LSOL = .TRUE.
 TAU = 0.0
 LAMBDA_D_K = 3.0

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 TIME = 0.07
 AEXX = 0.25
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LHFCALC = .TRUE.
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Panel (c)

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-9.7461529	3.5972250600000004	12.8374635
-9.6461529	1.1892217599999997	2.11661956
-9.5471529	0.009630709999999997	0.0007484099999999999
-9.4481529	3.2970000000000005e-05	0.0
-9.3481529	0.12061473000000003	1.6e-06
-9.2491529	0.8496528600000001	1.136e-05
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-6.4661529	0.010223300000000001	0.00018130000000000002
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-6.2671529	12.372030610000001	0.66164625
-6.1681529	2.19671403	0.13998219
-6.0691529	2.2963856999999996	0.10671711
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-4.2801529	0.23571599000000001	0.0052607800000000005
-4.1801529	0.05188886000000001	8.654000000000001e-05
-4.0811529	0.05151836	0.00016674
-3.9821529	0.26542661	0.0010729
-3.8821529	0.14434118	0.00765856
-3.7831529	6.18968948	1.3515304000000001
-3.6831529	12.096912699999999	1.9036372
-3.5841529	21.1302047	1.7934556
-3.4851529	19.197330800000003	2.3079976
-3.3851529	3.5098418899999997	0.40557306
-3.2861529	4.30144279	0.01283933
-3.1861529	12.315220649999999	0.0366446
-3.0871529	0.7960364200000001	0.0009501500000000001
-2.9881529	0.44499343	3.029e-05
-2.8881529	0.27886282999999995	2.221e-05
-2.7891529	0.45879586	5.4099999999999994e-05
-2.6901529	0.26204421	1.831e-05
-2.5901529	0.18289521	1.1839999999999998e-05
-2.4911529	0.11454989	4.66e-06

-2.3911529	0.11893226999999999	3.6199999999999996e-06
-2.2921529	0.0678118	2.1899999999999998e-06
-2.1931529	0.05092434	1.38e-06
-2.0931529	0.03662789	4.6499999999999995e-06
-1.9941529	0.16589969999999996	2.476e-05
-1.8941529	0.19307782000000007	1.9059999999999997e-05
-1.7951529	0.1570126	1.5629999999999998e-05
-1.6961529	0.12269292999999999	7.84e-06
-1.5961529	0.14430468999999999	4.340000000000001e-06
-1.4971529	0.08333315	1.485e-05
-1.3981529	0.0564382	9.43e-06
-1.2981529	0.08371015	5.799999999999999e-06
-1.1991529	0.09019632	2.6989999999999997e-05
-1.0991529	0.09918385	2.6739999999999998e-05
-1.0001529	0.17970796000000003	3.0900000000000006e-05
-0.9011529	0.16198243999999998	8.220000000000001e-06
-0.8011529	0.14324893000000002	1.168e-05
-0.7021529	0.13594188999999998	2.721e-05
-0.6021529	0.15610409	2.197e-05
-0.5031529	0.15240834	3.346e-05
-0.4041529	0.20545318999999998	2.414e-05
-0.3041529	0.18146515	3.7890000000000005e-05
-0.2051529	0.07837692000000002	1.586e-05
-0.1061529	0.11820362999999999	6.0500000000000005e-06
-0.0061529	0.09031759999999998	7.24e-06
0.0928471	0.09114754999999998	1.909e-05
0.1928471	0.32626805999999997	9.831000000000001e-05

0.2918471	0.20282863	1.777e-05
0.3908471	0.02695022	9.6e-07
0.4908471	0.024988680000000003	6e-07
0.5898471	0.02234188	6.499999999999999e-07
0.6898471	0.0905075	5.541e-05
0.7888471	0.14008118000000003	0.00010391
0.8878471	0.17999326000000002	4.458999999999999e-05
0.9878471	0.41562702000000007	4.085e-05
1.0868471	0.02731754	4.36200000000000006e-05
1.1858471	0.05432151	0.00014575
1.2858471	0.3400287500000001	8.740000000000001e-06
1.3848471	0.3841523200000001	1.576e-05
1.4848471	0.40758005	0.00012767
1.5838471	0.08935971999999999	5.69e-05
1.6828471	0.07246836	1.95800000000000002e-05
1.7828471	0.06453831000000002	2.434e-05
1.8818471	0.0029489100000000008	7.4e-07
1.9818471	0.27653842	5.01e-05
2.0808471	0.50788716	0.00060981
2.1798471	0.05622614	0.0001079
2.2798471	0.00935341	1.051e-05
2.3788471	0.15498153	0.00065321
2.4778471	0.36482706	0.00058599
2.5778471	1.15418803	0.00013103
2.6768471	0.49501232999999994	0.00280556
2.7768471	0.15898721000000002	0.01959128
2.8758471	0.018452930000000003	0.0026852499999999997

2.9748471	0.6523992499999999	0.09276896999999999
3.0748471	0.29046885	0.04129887
3.1738471	0.07614217000000001	0.0013344999999999997
3.2738471	0.21619528000000005	0.00417304
3.3728471	0.23258709	0.02559708
3.4718471	1.2212288199999999	0.09152855
3.5718471	0.6277092	0.02758558
3.6708471	0.56973465	0.057011509999999994
3.7698471	0.24385687999999994	0.042908169999999995
3.8698471	0.00312688	0.00040707000000000004
3.9688471	0.19311662999999996	0.00023891
4.0688471	0.6811968800000001	0.0024854300000000003
4.1678471	1.0866636	0.046217140000000004
4.2668471	1.10477706	0.10965429000000002
4.3668471	1.33009797	0.14372917
4.4658471	0.64191699	0.00707132
4.5658471	0.8747912899999999	0.05771756
4.6648471	0.8638442100000001	0.06625677
4.7638471	0.30585029	0.022549649999999997
4.8638471	0.31230842999999997	0.02469454
4.9628471	0.33359112	0.0015096
5.0618471	0.010788820000000003	1.398e-05
5.1618471	4.5e-07	0.0

Panel (d)

$E - E_{\mathrm{F}}$ / eV	H_2O *sp* pDOS / eV^{-1}	OH^- *sp* pDOS / eV^{-1}
-9.95399915	4.1999999999999995e-07	0.0

-9.86399915	0.0034955899999999994	0.0
-9.77399915	0.10429311000000001	1.8e-07
-9.68399915	0.04487569	6.999999999999999e-08
-9.59399915	0.20395917	3.8e-07
-9.50399915	0.7063474	1.3499999999999998e-06
-9.41399915	0.037678450000000016	6.999999999999999e-08
-9.32499915	8.34e-06	0.0
-9.23499915	0.00296217	0.0
-9.14499915	0.42044844000000003	1e-06
-9.05499915	0.5961099	1.42e-06
-8.96499915	0.32893262	1.25e-06
-8.87499915	0.6369826599999999	1.19e-06
-8.78499915	0.10260179000000001	5e-08
-8.69499915	0.00020003000000000002	0.0
-8.60599915	6.999999999999999e-08	0.0
-8.51599915	0.00314548	1e-08
-8.42599915	0.5005183100000001	1.95e-06
-8.33599915	1.5679848	3.72e-06
-8.24599915	0.3462060600000001	3.6000000000000005e-07
-8.15599915	0.37124821	1.11e-06
-8.06599915	0.9127290199999999	2.6000000000000005e-06
-7.97699915	0.16712584999999996	7.4e-07
-7.88699915	0.11597679999999998	5.8e-07
-7.79699915	0.06254044000000002	8e-08
-7.70699915	1.7490255500000003	2.11e-06
-7.61699915	2.23306311	5.63e-06
-7.52699915	3.3474051700000005	8.8e-06

-7.43699915	2.8881390400000004	3.4799999999999997e-06
-7.34699915	3.3837011500000003	5.17e-06
-7.25799915	0.32503702000000007	8.300000000000001e-07
-7.16799915	1.9153162599999998	4.65e-06
-7.07799915	4.5443054400000005	6.33e-06
-6.98799915	1.58475502	1.6900000000000001e-06
-6.89799915	0.7039330400000001	4.42e-06
-6.80799915	2.26620751	5.1899999999999994e-06
-6.71799915	2.8692296200000005	3.29e-06
-6.62899915	0.70485364	1.82e-06
-6.53899915	0.27589702	2.4e-07
-6.44899915	0.00881709	1.247e-05
-6.35899915	1.6727308900000002	0.01726527
-6.26899915	23.072317780000002	0.19086140000000001
-6.17899915	21.027864849999997	0.1410616
-6.08899915	21.2169599	0.664931
-5.99899915	19.396671729999998	0.477589
-5.90999915	1.2471791600000002	0.026612399999999998
-5.81999915	0.024235730000000004	1.2659999999999999e-05
-5.72999915	0.18049350000000003	0.00696205
-5.63999915	8.5854549	0.7258795699999999
-5.54999915	11.35875497	0.96290036
-5.45999915	0.40878950000000003	0.01942133
-5.36999915	0.19499665000000002	2.441e-05
-5.28099915	0.18471582	7.329999999999999e-06
-5.19099915	0.28405808999999993	9.72e-06
-5.10099915	0.19674367000000004	5.3e-06

-5.01099915	0.14878236999999997	4.3799999999999996e-06
-4.92099915	0.37001681000000003	8.54e-06
-4.83099915	0.28246538	1.1069999999999999e-05
-4.74099915	0.3463704000000001	1.419e-05
-4.65199915	0.16385316	9.16e-06
-4.56199915	0.7184651700000001	3.238e-05
-4.47199915	0.9846737799999999	8.12e-05
-4.38199915	0.6039784500000001	0.00010475999999999999
-4.29199915	0.5504706099999999	0.00018867000000000002
-4.20199915	0.22003730999999999	9.619000000000001e-05
-4.11199915	0.046971820000000004	6.279e-05
-4.02199915	0.06987487999999999	0.00028059
-3.93299915	0.19694657999999998	0.001547
-3.84299915	0.14546916	0.00239125
-3.75299915	0.32744366	0.3820793899999999
-3.66299915	2.71160204	5.3763203000000015
-3.57299915	2.69740356	8.118024199999999
-3.48299915	3.00973113	1.1294231
-3.39299915	8.024392209999998	1.547873
-3.30399915	4.84850248	1.4971568
-3.21399915	3.5407719600000007	0.5104528
-3.12399915	5.753569870000001	0.399761
-3.03399915	6.28274431	0.424838
-2.94399915	3.30038029	0.1564786
-2.85399915	0.96563712	0.0192354
-2.76399915	0.49216891999999995	0.0009638600000000001
-2.67399915	0.5296218199999999	0.00942088

-2.58499915	3.24172992	0.3026599
-2.49499915	6.619243020000001	0.6252464
-2.40499915	5.2493973700000005	0.4015764
-2.31499915	5.8131731900000005	0.4301759
-2.22499915	6.89835708	0.5743163
-2.13499915	5.01946558	0.4580179
-2.04499915	2.7077211200000004	0.20018020999999997
-1.95599915	1.53385179	0.08540148
-1.86599915	4.76315601	0.26227135
-1.77599915	5.57165156	0.27353683
-1.68599915	6.3214749999999995	0.22436201
-1.59599915	2.67752458	0.07075266000000001
-1.50599915	0.35605307999999997	0.00503105
-1.41599915	0.09748325000000001	0.00056254
-1.32599915	0.07256488000000001	0.00017912
-1.23699915	0.06778719000000001	5.198000000000001e-05
-1.14699915	0.047440359999999994	8.651e-05
-1.05699915	0.15930956	0.0008231299999999999
-0.96699915	0.24613702999999995	0.0011418200000000002
-0.87699915	9.592202689999999	0.058053549999999995
-0.78699915	14.67592341	0.09362989999999999
-0.69699915	10.886030710000002	0.0840039
-0.60799915	1.2357845200000002	0.01262908
-0.51799915	12.847817759999998	0.1693286
-0.42799915	5.80431475	0.1266691
-0.33799915	14.701306	0.969282
-0.24799915	11.6904075	3.972231

-0.15799915	3.1543399699999997	1.8911672000000004
-0.06799915	8.77994996	12.0154676
0.02200085	8.20149139	7.496955900000001
0.11100085	0.23745009	0.15589315
0.20100085	0.18720317	0.00048144999999999997
0.29100085	0.31568669	0.0025093199999999998
0.38100085	0.28594545	0.00219253
0.47100085	0.06850888999999999	0.00120171
0.56100085	0.05492755	6e-05
0.65100085	0.018796669999999998	1.36e-05
0.74000085	0.041058149999999995	4.358e-05
0.83000085	0.02246104	3.2749999999999996e-05
0.92000085	0.20041139000000002	0.00045567000000000003
1.01000085	0.48518669000000003	0.00072268
1.10000085	0.23300636000000002	0.0001753
1.19000085	0.1398161	0.00035491
1.28000085	0.03994904	4.045e-05
1.37000085	0.34307251	2.094e-05
1.45900085	0.39251142	9.771e-05
1.54900085	0.31088922999999996	0.00011102
1.63900085	0.08653896000000001	6.77e-05
1.72900085	0.26821532000000003	0.00030579999999999995
1.81900085	0.16159021	0.00025641
1.90900085	0.07025856000000001	2.4770000000000002e-05
1.99900085	0.06925618999999998	7.156e-05
2.08800085	0.2757713899999999	5.264e-05
2.17800085	0.58998486	1.8719999999999997e-05

2.26800085	0.03920031000000001	1.1600000000000001e-06
2.35800085	0.020225440000000004	7.42e-06
2.44800085	0.21646092999999997	0.00022442
2.53800085	0.13287352	0.00013563
2.62800085	0.17976749	1.85e-05
2.71800085	1.1134876200000001	0.00012096
2.80700085	0.83920176	0.0004826
2.89700085	0.25996934000000005	0.00018166000000000002
2.98700085	0.10180748	1.8829999999999998e-05
3.07700085	0.0010802099999999999	2.3000000000000002e-07
3.16700085	3.0000000000000004e-08	0.0
3.25700085	0.0	0.0
3.34700085	0.0	0.0
3.43600085	2.7e-07	0.0
3.52600085	0.00474004	1.25e-06
3.61600085	0.3537782099999999	8.906e-05
3.70600085	0.6703266000000001	0.00081759
3.79600085	0.19120262999999998	0.0005519300000000001
3.88600085	0.00180807	5.57e-06
3.97600085	7.887e-05	1.4999999999999997e-07
4.06600085	0.06911171	0.00011006
4.15500085	0.7062678299999999	0.0006307699999999999
4.24500085	0.55191239	0.0001742
4.33500085	0.29617749	7.688999999999999e-05
4.42500085	0.24839700000000003	4.113e-05
4.51500085	0.046515499999999994	1.8040000000000003e-05
4.60500085	0.36001163	0.00012301

4.69500085	0.5329338499999999	0.00032166000000000003
4.78400085	0.42006199999999994	0.00249046
4.87400085	0.47826605000000005	0.01970528
4.96400085	0.47210958000000003	0.004234020000000001
5.05400085	0.5007322000000001	0.0482396
5.14400085	0.8348869999999999	0.11409239
5.23400085	0.53715391	0.006016779999999999
5.32400085	0.19244079999999997	0.00033845999999999995
5.41300085	0.22918191999999998	0.00077732
5.50300085	0.72674762	0.07998453999999999
5.59300085	1.0223443200000002	0.1156495
5.68300085	0.7455237899999999	0.00245604
5.77300085	0.2115035	7.609e-05
5.86300085	0.14254363999999997	6.837999999999999e-05
5.95300085	0.59260197	0.00077888
6.04300085	0.5904962	0.00084481
6.13200085	0.028186239999999998	4.0480000000000005e-05
6.22200085	7.46e-06	0.0

Panel (e)

$E - E_{\mathrm{F}}$ / eV	H_2O *sp* pDOS / eV^{-1}	H_3O^+ *sp* pDOS / eV^{-1}
-11.50953459	1.4e-06	9.64e-06
-11.39653459	0.11273455	0.77245616
-11.28253459	2.14157164	14.246398019999999
-11.16853459	3.196449280000001	13.022452600000001
-11.05453459	0.21504577000000002	0.8511124499999998
-10.94053459	0.0007084499999999999	1.4000000000000001e-05

-10.82653459	0.102394	1.4900000000000001e-06
-10.71353459	0.04006817	5.599999999999999e-07
-10.59953459	0.6297604099999999	8.34e-06
-10.48553459	0.23385444999999996	3.0300000000000002e-06
-10.37153459	6.750000000000001e-05	3.0000000000000004e-08
-10.25753459	0.76343918	0.0045798
-10.14353459	26.01201063	0.1688903
-10.02953459	25.50348822	0.4452596
-9.91653459	19.364502249999997	0.3177869
-9.80253459	18.332407949999997	0.270875
-9.68853459	0.19291589999999997	0.00281422
-9.57453459	3.900000000000001e-07	0.0
-9.46053459	0.022998069999999995	4.3e-07
-9.34653459	1.6964288800000002	3.6270000000000003e-05
-9.23253459	0.46377132	1.073e-05
-9.11953459	0.5613556000000001	8.26e-06
-9.00553459	0.5768857900000001	8.51e-06
-8.89153459	0.019900240000000007	1.2999999999999997e-07
-8.77753459	0.013795160000000002	1e-07
-8.66353459	2.3462039999999997	2.026e-05
-8.54953459	4.44892443	2.833e-05
-8.43653459	4.11213731	1.0060000000000002e-05
-8.32253459	0.50359576	1.99e-06
-8.20853459	1.14171955	8.930000000000001e-06
-8.09453459	4.818313080000001	2.1890000000000002e-05
-7.98053459	1.06389744	5.38e-06
-7.86653459	1.5446605899999997	9.34e-06

-7.75253459	2.6519257599999997	6.565e-05
-7.63953459	3.1585789899999996	0.12546068999999999
-7.52553459	11.580041859999998	0.5967563
-7.41153459	1.1467063100000001	0.05606179
-7.29753459	3.7440468200000003	0.18274017
-7.18353459	8.031407130000002	0.5608713999999999
-7.06953459	13.753051480000002	1.0281813
-6.95553459	3.7040494499999994	0.33443331
-6.84253459	0.18507178999999999	0.00145691
-6.72853459	0.07176946	2.546e-05
-6.61453459	0.46319228	0.056765220000000005
-6.50053459	3.6333082099999996	0.40584020000000004
-6.38653459	7.467587549999999	0.7432593
-6.27253459	5.5571659	0.993756
-6.15953459	5.723086	2.71448
-6.04553459	2.20064206	1.8014835000000002
-5.93153459	2.5442352500000003	1.2460053999999998
-5.81753459	5.5642217	4.49308
-5.70353459	1.0054875099999998	1.0237594
-5.58953459	0.2982395300000001	0.0019003200000000003
-5.47553459	0.24721767000000003	6.093e-05
-5.36253459	0.7957476699999999	0.00014008
-5.24853459	0.5783013	9.829e-05
-5.13453459	0.3337816200000001	0.0007151500000000001
-5.02053459	4.027631230000001	0.8317355
-4.90653459	11.01339685	2.011755
-4.79253459	17.0635064	1.3425582999999999

-4.67953459	19.742497200000003	1.9768270000000001
-4.56553459	8.415897600000001	0.32915990000000006
-4.45153459	9.241434309999999	0.07420155
-4.33753459	0.23427676000000003	0.0002813
-4.22353459	0.26527346000000007	1.465e-05
-4.10953459	0.19166436000000006	1.182e-05
-3.99553459	0.28734296	1.807e-05
-3.88253459	0.3504125900000001	1.2819999999999998e-05
-3.76853459	0.29371978	2.863e-05
-3.65453459	0.18728329999999996	1.288e-05
-3.54053459	0.15888247000000005	8.1e-06
-3.42653459	0.5262957999999999	1.9600000000000002e-05
-3.31253459	0.4359785799999999	1.378e-05
-3.19853459	0.17202673	8.26e-06
-3.08553459	0.19684647	2.9700000000000004e-06
-2.97153459	0.07506178999999999	1.37e-06
-2.85753459	0.16687857	5.19e-06
-2.74353459	0.06232129	3.6099999999999993e-06
-2.62953459	0.14436846000000003	4.849999999999999e-06
-2.51553459	0.21481189	1.23e-05
-2.40253459	0.11033449999999997	1.017e-05
-2.28853459	0.11459637999999997	5.73e-06
-2.17453459	0.16549842	6.06e-06
-2.06053459	0.09493614	8.57e-06
-1.94653459	0.019614970000000002	2.94e-06
-1.83253459	0.036502549999999995	2.02e-06
-1.71853459	0.025737990000000002	6.000000000000001e-07

-1.60553459	0.09341508000000001	9.570000000000002e-06
-1.49153459	0.12015798999999999	8.88e-06
-1.37753459	0.18514492	1.887e-05
-1.26353459	0.13736868	1.2929999999999998e-05
-1.14953459	0.16542693000000006	1.2230000000000001e-05
-1.03553459	0.06908134	3.4e-06
-0.92153459	0.10660998000000001	7.25e-06
-0.80853459	0.15536514	1.167e-05
-0.69453459	0.11357903999999999	2.092e-05
-0.58053459	0.10139631999999998	1.358e-05
-0.46653459	0.08935373999999999	4.27e-06
-0.35253459	0.06126186000000001	2.68e-06
-0.23853459	0.11815787	1.5e-06
-0.12553459	0.07936175999999999	1.3899999999999998e-06
-0.01153459	0.024419410000000003	5.2e-06
0.10246541	0.05275963	2.7340000000000003e-05
0.21646541	0.17835852999999996	1.47e-05
0.33046541	0.26943039	5.059e-05
0.44446541	0.11862112	1.1309999999999998e-05
0.55846541	0.03616227	1.19e-06
0.67146541	0.00438008	7.999999999999999e-08
0.78546541	0.028539039999999995	9.3e-07
0.89946541	0.11936831999999999	6.226e-05
1.01346541	0.12921187999999997	6.141999999999999e-05
1.12746541	0.13134327	1.0899999999999999e-05
1.24146541	0.37839955000000003	5.079e-05
1.35446541	0.09342820000000002	8.982e-05

1.46846541	0.016515810000000002	3.2279999999999996e-05
1.58246541	0.24660705999999996	3.19e-06
1.69646541	0.27941144	2.97e-06
1.81046541	0.27187061	2.2460000000000002e-05
1.92446541	0.24526944	0.00010360999999999999
2.03846541	0.06429263	4.1269999999999996e-05
2.15146541	0.017097379999999995	3.3300000000000003e-06
2.26546541	0.09207753000000002	3.170999999999999e-05
2.37946541	0.38952102999999993	0.00027966
2.49346541	0.32124178	0.00019086000000000003
2.60746541	0.033240189999999996	2.56e-06
2.72146541	0.0050273800000000006	3.2659999999999996e-05
2.83546541	0.13857572	0.00065635
2.94846541	0.07257430999999999	0.00010343
3.06246541	0.25091184	4.649e-05
3.17646541	1.2435875100000002	0.00023603000000000003
3.29046541	0.30138669000000007	0.01240758
3.40446541	0.04323408	0.004513680000000001
3.51846541	0.42817901	0.06262633000000001
3.63146541	0.23899841	0.03292449
3.74546541	0.17986025	0.0034358300000000004
3.85946541	0.01361287	0.00062819
3.97346541	0.4884395	0.06041552
4.08746541	0.3492211	0.02765847
4.20146541	0.9134969599999999	0.046158370000000004
4.31546541	0.23792095	0.035897029999999996
4.42846541	0.04642683	0.0043143899999999995

4.54246541	0.09039842999999999	0.012780530000000002
4.65646541	0.08282083999999999	0.011030519999999999
4.77046541	0.7391249700000001	0.04151571
4.88446541	0.5395676	0.058306920000000005
4.99846541	0.5897549999999999	0.056807819999999995
5.11246541	0.6623968	0.05541531
5.22546541	0.39522681	0.026094759999999998
5.33946541	0.19287700999999996	0.00875813
5.45346541	0.3321184	0.022280679999999997
5.56746541	0.32370514	0.030618329999999996
5.68146541	0.30778915	0.026294059999999998
5.79546541	0.14308757999999996	0.01227514
5.90846541	0.23987513	0.02477913
6.02246541	0.14573226	0.01359392
6.13646541	0.012215710000000001	0.0005704799999999999
6.25046541	0.056252300000000005	0.0024242
6.36446541	0.0013242600000000003	5.707e-05

Panel (f)

$E - E_{\mathrm{F}}$ / eV	H_2O *sp* pDOS / eV^{-1}	OH^- *sp* pDOS / eV^{-1}
-10.7246741	0.00268076	0.0
-10.6196741	0.1086268	2e-07
-10.5136741	0.025731310000000007	4e-08
-10.4086741	0.44906564	9.1e-07
-10.3036741	0.39566466	7.8e-07
-10.1976741	0.0009477800000000001	0.0
-10.0926741	7.329999999999999e-06	0.0

-9.9866741	0.08240113000000003	2.1e-07
-9.8816741	0.7880053199999999	1.9699999999999998e-06
-9.7766741	0.15332314000000002	5.900000000000001e-07
-9.6706741	0.6274166000000002	1.72e-06
-9.5656741	0.21510159000000004	1.3e-07
-9.4606741	0.00050529	0.0
-9.3546741	6e-08	0.0
-9.2496741	0.009766629999999998	4e-08
-9.1446741	0.89946269	3.33e-06
-9.0386741	1.20285504	2.02e-06
-8.9336741	0.13153204000000002	2.7e-07
-8.8276741	0.9995175799999999	2.82e-06
-8.7226741	0.07681040000000001	2.2e-07
-8.6176741	0.0368975	2e-07
-8.5116741	0.6426276799999999	1.3399999999999999e-06
-8.4066741	2.75448635	3.8400000000000005e-06
-8.3016741	3.8188096299999996	7.1299999999999995e-06
-8.1956741	3.6250950200000003	6.04e-06
-8.0906741	0.81745815	2.3500000000000004e-06
-7.9856741	0.5374593900000001	1.4499999999999999e-06
-7.8796741	4.42235853	7.81e-06
-7.7746741	2.05837363	3.01e-06
-7.6686741	0.48862918999999994	9.800000000000001e-07
-7.5636741	2.5062970899999995	3.55e-06
-7.4586741	1.61720402	2.4400000000000004e-06
-7.3526741	1.17790824	0.0028761800000000003
-7.2476741	21.464696729999996	0.09452680000000001

-7.1426741	16.221034539999998	0.0319095
-7.0366741	5.26210466	0.163652
-6.9316741	25.81012657	0.726077
-6.8266741	6.075350890000001	0.148742
-6.7206741	0.11030902999999996	0.00015239000000000002
-6.6156741	0.039502270000000006	3.29e-06
-6.5096741	0.32820812	0.019278220000000002
-6.4046741	13.24865786	0.9032882599999998
-6.2996741	4.07987583	0.27276233
-6.1936741	0.19263887999999998	0.00019288999999999998
-6.0886741	0.06967519	3.87e-06
-5.9836741	0.10660166000000001	2.99e-06
-5.8776741	0.2535302	5.63e-06
-5.7726741	0.19210323999999998	4.16e-06
-5.6676741	0.13321319	4.7399999999999995e-06
-5.5616741	0.3378066899999999	1.0490000000000001e-05
-5.4566741	0.1390091	2.4500000000000003e-06
-5.3506741	0.49472902	1.762e-05
-5.2456741	0.77050187	3.163e-05
-5.1406741	0.59320958	3.429e-05
-5.0346741	0.38660183000000004	5.1599999999999994e-05
-4.9296741	0.4055279599999999	0.00011943000000000001
-4.8246741	0.21348115999999998	0.00012706
-4.7186741	0.04669550000000001	6.836e-05
-4.6136741	0.03720495	0.0009222
-4.5086741	3.6771937400000003	0.36265929999999996
-4.4026741	10.605888570000001	0.7946120999999999

-4.2976741	1.34642256	0.06083557999999999
-4.1916741	3.63566424	0.5536265
-4.0866741	6.0549923	1.2861012
-3.9816741	4.02759083	3.9589798000000003
-3.8756741	4.2078443000000005	6.532800099999999
-3.7706741	2.01501378	2.3395451
-3.6656741	0.28941318	0.02702072
-3.5596741	0.27722642	0.00362595
-3.4546741	1.6794255400000002	0.1488152
-3.3496741	6.83925421	0.56558
-3.2436741	5.9608364300000005	0.449566
-3.1386741	4.86343498	0.3959505
-3.0326741	6.00880754	0.520296
-2.9276741	4.9168921999999995	0.4432716
-2.8226741	2.41948856	0.16839939999999998
-2.7166741	4.022771339999999	0.16935868999999998
-2.6116741	5.41618779	0.20504921
-2.5066741	6.14567319	0.16511652
-2.4006741	1.83315036	0.03445768
-2.2956741	0.19260512999999999	0.00130934
-2.1906741	0.13138331	0.00022423
-2.0846741	0.18395288999999998	0.00030071
-1.9796741	0.10998709000000004	0.00046693
-1.8736741	0.68736178	0.0013814699999999999
-1.7686741	18.28558207	0.0493738
-1.6636741	11.51711513	0.05677619999999999
-1.5576741	0.20666993	0.0009564100000000001

-1.4526741	9.223059680000002	0.0679549
-1.3476741	7.7963096100000016	0.0589365
-1.2416741	13.09435625	0.0909069
-1.1366741	1.15011325	0.013450060000000002
-1.0316741	10.360411070000001	0.32257499999999995
-0.9256741	4.35279809	0.13563260000000002
-0.8206741	0.08628753	0.00136437
-0.7146741	0.14724352000000002	0.0020003399999999998
-0.6096741	0.17695741000000004	0.00465262
-0.5046741	0.17184283	0.036800950000000006
-0.3986741	2.33620543	6.714410160000001
-0.2936741	6.24160417	15.214988100000001
-0.1886741	0.80043687	1.4977339900000002
-0.0826741	0.07550553000000002	0.0009781299999999998
0.0223259	0.048741780000000005	0.00011753999999999999
0.1273259	0.01399746	8.37e-06
0.2333259	0.09439792999999999	3.137e-05
0.3383259	0.22293082	0.00034810999999999995
0.4443259	0.23162994	0.00045628
0.5493259	0.17648299999999997	0.00013501
0.6543259	0.12391548000000001	0.00047518999999999995
0.7603259	0.009556619999999998	6.095e-05
0.8653259	0.02575831	4.4e-06
0.9703259	0.02607446	4.2999999999999995e-06
1.0763259	0.034060639999999996	1.266e-05
1.1813259	0.07962165	5.204e-05
1.2863259	0.49012445	0.00038492

1.3923259	0.28674155	0.00024237
1.4973259	0.032695539999999995	4.229e-05
1.6033259	0.14571631000000002	0.00021494000000000003
1.7083259	0.20743081000000005	2.4120000000000003e-05
1.8133259	0.33410067000000004	2.0490000000000002e-05
1.9193259	0.34532291000000004	8.569e-05
2.0243259	0.04112224999999999	2.8879999999999998e-05
2.1293259	0.01315142	8.890000000000001e-06
2.2353259	0.19533746999999999	0.0001309
2.3403259	0.22552371000000002	0.00024240999999999998
2.4453259	0.059173699999999996	4.268e-05
2.5513259	0.3798312100000001	3.537e-05
2.6563259	0.46640177000000005	6.151e-05
2.7623259	0.028702960000000003	1.3939999999999999e-05
2.8673259	0.0213639	2.74e-06
2.9723259	0.19100827	0.00015039
3.0783259	0.1213322	9.811999999999999e-05
3.1833259	0.022675480000000005	5.87e-06
3.2883259	0.3796040300000001	1.0209999999999999e-05
3.3943259	0.9026309100000001	0.00025217
3.4993259	0.53885956	0.00024872
3.6043259	0.2658133900000001	7.779e-05
3.7103259	0.06767477	9.679999999999999e-06
3.8153259	9.684e-05	0.0
3.9213259	0.0	0.0
4.0263259	0.0	0.0
4.1313259	0.0	0.0

4.2373259	0.00184749	2.2999999999999996e-06
4.3423259	0.18870343	0.00038155
4.4473259	0.5634517299999999	0.00148995
4.5533259	0.17846308	0.0005172499999999999
4.6583259	0.039796299999999986	0.0012325699999999999
4.7633259	0.03734995	0.00120996
4.8693259	0.13545392	0.0005221199999999999
4.9743259	0.07377726	0.00033791999999999996
5.0803259	0.22948589000000005	0.00054511
5.1853259	0.24423672	0.0025467700000000003
5.2903259	0.15328742000000006	0.0020623399999999997
5.3963259	0.06556859000000002	0.00095856
5.5013259	0.11009136	0.006341449999999999
5.6063259	0.13826276	0.014950890000000001
5.7123259	0.18513728	0.02069284
5.8173259	0.54509394	0.0655588
5.9223259	0.41990221000000005	0.04866165
6.0283259	0.08793721000000002	0.00497218
6.1333259	0.25876665	0.02671413
6.2393259	0.29273004	0.04458817
6.3443259	0.1550761	0.01901917
6.4493259	0.12365126999999998	0.00889545
6.5553259	0.11076337000000001	0.02208996
6.6603259	0.07367335	0.01224516
6.7653259	0.15567955	0.017667369999999998
6.8713259	0.15811748	0.024404319999999997
6.9763259	0.1709036	0.03734311

7.0813259	0.11173730999999999	0.03018078
7.1873259	0.21237391	0.042028579999999996
7.2923259	0.11656983	0.02130487
7.3983259	0.07019713000000001	0.019346330000000002
7.5033259	0.203149	0.0312812
7.6083259	0.18026430999999998	0.028381539999999997
7.7143259	0.09093138	0.020922879999999998
7.8193259	0.10677447999999999	0.035840250000000004
7.9243259	0.04665941	0.010029010000000001
8.0303259	0.04408106	0.00805237
8.1353259	0.00085126	0.00013906

Figure 2

Panel (a)

$E - E_\mathrm{F}$ / eV	H_2O *sp* pDOS / eV^{-1}	OH^- *sp* pDOS / eV^{-1}
-9.96175543	1.7999999999999997e-07	0.0
-9.87175543	0.00212784	0.0
-9.78175543	0.09455905	1.7000000000000001e-07
-9.69175543	0.05552442000000001	9e-08
-9.60175543	0.15343872999999997	2.9e-07
-9.51175543	0.73759639	1.39e-06
-9.42175543	0.056767970000000015	1.0000000000000001e-07
-9.33175543	1.977e-05	0.0
-9.24175543	0.00159692	0.0
-9.15175543	0.34590037	8.200000000000001e-07
-9.06275543	0.66259606	1.57e-06

-8.97275543	0.2881508	1.0900000000000002e-06
-8.88275543	0.6550725300000001	1.3299999999999998e-06
-8.79275543	0.13332823	8e-08
-8.70275543	0.00039135	0.0
-8.61275543	0.0	0.0
-8.52275543	0.0017354599999999999	1e-08
-8.43275543	0.40515772000000005	1.58e-06
-8.34275543	1.5765903499999996	3.91e-06
-8.25375543	0.43062635000000005	4.4e-07
-8.16375543	0.29841529999999994	9.000000000000001e-07
-8.07375543	0.96812755	2.7299999999999997e-06
-7.98375543	0.16940642000000006	7.1e-07
-7.89375543	0.13212772999999997	6.4e-07
-7.80375543	0.04119963000000002	5e-08
-7.71375543	1.58751383	1.88e-06
-7.62375543	2.19191045	5.060000000000001e-06
-7.53375543	3.3929402299999993	8.98e-06
-7.44375543	2.737331850000001	3.4800000000000006e-06
-7.35475543	3.611404	5.19e-06
-7.26475543	0.40410619000000003	9.800000000000001e-07
-7.17475543	1.6553798700000002	4.07e-06
-7.08475543	4.534809040000001	6.55e-06
-6.99475543	1.85192337	1.96e-06
-6.90475543	0.6024357300000001	3.87e-06
-6.81475543	2.188236869999999	5.48e-06
-6.72475543	2.9647717100000004	3.29e-06
-6.63475543	0.75680335	1.98e-06

-6.54475543	0.31979087	2.8e-07
-6.45575543	0.01022475	1.574e-05
-6.36575543	1.9627390000000002	0.018442280000000002
-6.27575543	24.637505239999996	0.1749899
-6.18575543	19.1237652	0.11244699999999999
-6.09575543	20.15414743	0.65957
-6.00575543	20.29155168	0.511818
-5.91575543	1.4117081500000002	0.030292979999999997
-5.82575543	0.025349779999999995	0.00011538
-5.73575543	1.8174077199999998	0.13193119999999997
-5.64575543	15.86337995	1.19826074
-5.55675543	2.91994372	0.21385148
-5.46675543	0.16914729999999997	0.00031804
-5.37675543	0.20232421999999997	1.2309999999999999e-05
-5.28675543	0.18355085999999995	4.840000000000001e-06
-5.19675543	0.2759083	7.350000000000001e-06
-5.10675543	0.20895381000000002	4.57e-06
-5.01675543	0.14412110999999997	4.0299999999999995e-06
-4.92675543	0.35389733	7.599999999999999e-06
-4.83675543	0.2947782299999999	1.075e-05
-4.74775543	0.34270795000000004	1.3209999999999999e-05
-4.65775543	0.16891836	9.02e-06
-4.56775543	0.67130596	2.7630000000000005e-05
-4.47775543	1.00310014	7.248000000000001e-05
-4.38775543	0.6106848699999998	9.213000000000001e-05
-4.29775543	0.5619759399999998	0.00016636
-4.20775543	0.2376319	9.206000000000001e-05

-4.11775543	0.05016972000000001	5.051e-05
-4.02775543	0.06712441	0.00021082999999999999
-3.93775543	0.18571331999999996	0.00108176
-3.84875543	0.15711170000000002	0.0012600900000000002
-3.75875543	0.15213364000000001	0.052378020000000004
-3.66875543	1.85984929	2.2885207
-3.57875543	4.019629259999999	6.6972553999999995
-3.48875543	3.8212749200000005	4.4740193999999995
-3.39875543	6.70873575	1.9181190000000001
-3.30875543	5.11483541	2.193319
-3.21875543	3.96414434	0.7630688999999999
-3.12875543	5.66126223	0.483721
-3.03875543	6.2009682800000006	0.476975
-2.94975543	2.98412391	0.1450197
-2.85975543	0.9482282200000001	0.01861905
-2.76975543	0.49747389	0.0010616
-2.67975543	0.5630257599999999	0.01314953
-2.58975543	3.6603649799999998	0.3463103
-2.49975543	6.75373551	0.6283046
-2.40975543	5.17537787	0.387556
-2.31975543	6.98591477	0.5188658
-2.22975543	7.493134199999999	0.592544
-2.14075543	3.87279753	0.302474
-2.05075543	2.3254959	0.13564853000000002
-1.96075543	0.9736017100000001	0.04479817999999999
-1.87075543	4.97591653	0.25075295000000003
-1.78075543	5.98694869	0.25351778

-1.69075543	6.3581913100000005	0.18881802
-1.60075543	2.18466991	0.044759400000000005
-1.51075543	0.25145714999999996	0.00224813
-1.42075543	0.09605042	0.00052497
-1.33075543	0.07366236999999999	0.00019005999999999998
-1.24175543	0.06903584	5.12e-05
-1.15175543	0.04568275000000001	7.463000000000001e-05
-1.06175543	0.15843943999999996	0.00080409
-0.97175543	0.39600832	0.0019004500000000001
-0.88175543	11.615949270000005	0.06045791
-0.79175543	13.956187340000001	0.0817518
-0.70175543	9.559645830000001	0.067037
-0.61175543	0.9713149200000001	0.00901567
-0.52175543	12.46830482	0.15131989999999998
-0.43175543	8.49648972	0.23830880000000002
-0.34275543	18.0094235	1.237552
-0.25275543	11.2729733	1.221896
-0.16275543	0.77063166	0.1807433
-0.07275543	5.10996646	8.8757546
0.01724457	8.72037089	14.8194776
0.10724457	0.28277806	0.42169803000000006
0.19724457	0.17733833000000002	0.00046439
0.28724457	0.31045883999999996	0.00246761
0.37724457	0.28889177	0.00225034
0.46624457	0.07182502	0.00130127
0.55624457	0.05343794000000001	6.029e-05
0.64624457	0.020235959999999997	1.416e-05

0.73624457	0.039616	4.247999999999999e-05
0.82624457	0.02318472	3.393e-05
0.91624457	0.18845380000000003	0.00045463000000000003
1.00624457	0.48047267	0.00076852
1.09624457	0.24547522000000002	0.00018329999999999998
1.18624457	0.14056901	0.000371
1.27624457	0.038068050000000006	4.697e-05
1.36524457	0.32994437000000004	2.0379999999999998e-05
1.45524457	0.3960858899999999	9.921e-05
1.54524457	0.32093945000000007	0.00011732999999999999
1.63524457	0.0837118	6.621e-05
1.72524457	0.26707448	0.00031129000000000004
1.81524457	0.16557393000000004	0.00027214
1.90524457	0.07030531	2.583e-05
1.99524457	0.06869389999999999	7.315e-05
2.08524457	0.25778692999999997	5.4609999999999994e-05
2.17524457	0.6031574199999999	1.9750000000000002e-05
2.26424457	0.045407750000000004	1.38e-06
2.35424457	0.01839543	7.12e-06
2.44424457	0.21466121999999996	0.00022849
2.53424457	0.13417478	0.00014145
2.62424457	0.16584212999999998	1.871e-05
2.71424457	1.0995159799999998	0.00012027
2.80424457	0.8586080199999999	0.0004938
2.89424457	0.26439702000000004	0.00019018
2.98424457	0.10560938	1.986e-05
3.07324457	0.001226	2.6999999999999996e-07

3.16324457	3.0000000000000004e-08	0.0
3.25324457	0.0	0.0
3.34324457	0.0	0.0
3.43324457	2.1000000000000003e-07	0.0
3.52324457	0.004158880000000001	1.16e-06
3.61324457	0.33900975	8.989000000000001e-05
3.70324457	0.68148638	0.00083202
3.79324457	0.19396762999999997	0.00056797
3.88324457	0.0018590399999999997	5.849999999999999e-06
3.97224457	7.373e-05	1.4999999999999997e-07
4.06224457	0.06618409	0.00011124
4.15224457	0.69585149	0.0006420600000000001
4.24224457	0.5591445500000001	0.00017675000000000001
4.33224457	0.29400727	7.841e-05
4.42224457	0.2534522	4.279e-05
4.51224457	0.044408460000000004	1.687e-05
4.60224457	0.35504736	0.00012294999999999998
4.69224457	0.5282787400000001	0.00032058000000000005
4.78224457	0.43393934	0.0029146300000000005
4.87124457	0.47872882	0.01961486
4.96124457	0.46890288	0.00380342
5.05124457	0.52953017	0.05386236
5.14124457	0.8048488899999999	0.10840916
5.23124457	0.5362933299999999	0.00505539
5.32124457	0.191189	0.00034271999999999997
5.41124457	0.22870852	0.00096281
5.50124457	0.75742206	0.08689559999999999

5.59124457	0.99049822	0.10817009999999998
5.68124457	0.74798712	0.00195509
5.77024457	0.21019986	7.659999999999999e-05
5.86024457	0.14506921999999997	6.942999999999999e-05
5.95024457	0.5908443099999999	0.00078542
6.04024457	0.5902367500000001	0.00085352
6.13024457	0.028060619999999994	4.0709999999999995e-05
6.22024457	7.38e-06	0.0

Panel (b)

$E - E_{\mathrm{F}}$ / eV	H_2O *sp* pDOS / eV^{-1}	OH^- *sp* pDOS / eV^{-1}
-9.96861971	1.7999999999999997e-07	0.0
-9.87861971	0.0022732	0.0
-9.78861971	0.09658678000000001	1.8e-07
-9.69861971	0.05366906000000002	1.0000000000000001e-07
-9.60761971	0.16871144000000002	3.5e-07
-9.51761971	0.7314844499999998	1.4900000000000001e-06
-9.42761971	0.04905747	1.0000000000000001e-07
-9.33661971	1.3749999999999999e-05	0.0
-9.24661971	0.0023343699999999997	0.0
-9.15661971	0.3952891	1.02e-06
-9.06661971	0.6207878	1.6000000000000001e-06
-8.97561971	0.32177859000000003	1.31e-06
-8.88561971	0.6431397799999997	1.3099999999999997e-06
-8.79561971	0.10695233	6e-08
-8.70561971	0.00021471	0.0
-8.61461971	6.999999999999999e-08	0.0

-8.52461971	0.00358403	1e-08
-8.43461971	0.52844468	2.2e-06
-8.34461971	1.5670554200000002	3.9399999999999995e-06
-8.25361971	0.32049837	3.6000000000000005e-07
-8.16361971	0.4077859700000001	1.32e-06
-8.07361971	0.8838293899999998	2.72e-06
-7.98361971	0.14850903999999995	7.3e-07
-7.89261971	0.12421565999999999	6.8e-07
-7.80261971	0.08717201000000002	1.2e-07
-7.71261971	1.8661730800000003	2.5e-06
-7.62261971	2.25716344	6.539999999999999e-06
-7.53161971	3.2631628200000002	9.13e-06
-7.44161971	3.0002655900000006	3.8e-06
-7.35161971	3.23426362	5.64e-06
-7.26161971	0.2973425900000001	8.9e-07
-7.17061971	2.2166271399999995	5.88e-06
-7.08061971	4.484766560000001	6.72e-06
-6.99061971	1.3173554799999998	1.65e-06
-6.90061971	0.8338689399999999	5.3400000000000005e-06
-6.80961971	2.40247168	5.96e-06
-6.71961971	2.664845230000001	3.88e-06
-6.62961971	0.6742546199999999	2.23e-06
-6.53961971	0.29037233999999995	0.0006671299999999999
-6.44861971	9.79477445	0.0727594
-6.35861971	29.39449481	0.138082
-6.26861971	9.961522270000001	0.17754109999999998
-6.17761971	25.87836201	0.757495

-6.08761971	11.988591069999998	0.29198399999999997
-5.99761971	0.18202949999999998	0.00371098
-5.90761971	0.06341138	2.783e-05
-5.81661971	0.94019293	0.07183759
-5.72661971	14.95368603	1.1590058300000001
-5.63661971	4.464270599999999	0.33583759
-5.54661971	0.09115087	0.000863
-5.45561971	0.19755415999999992	1.015e-05
-5.36561971	0.18550037	6.58e-06
-5.27561971	0.1875713	4.39e-06
-5.18561971	0.29233977000000005	7.75e-06
-5.09461971	0.17870392999999998	4.33e-06
-5.00461971	0.15603297	4.99e-06
-4.91461971	0.38909837000000014	1.0850000000000001e-05
-4.82461971	0.26819306	1.335e-05
-4.73361971	0.3454824	1.77e-05
-4.64361971	0.17489935999999998	1.091e-05
-4.55361971	0.8289026800000002	4.591e-05
-4.46361971	0.9161110399999999	0.00010051
-4.37261971	0.5835649799999999	0.00013693
-4.28261971	0.5111205400000001	0.00023258
-4.19261971	0.17781129	9.612000000000001e-05
-4.10261971	0.04196517	9.220999999999999e-05
-4.01161971	0.07798517	0.00047680000000000004
-3.92161971	0.22895484000000002	0.0028165499999999997
-3.83161971	0.25948535	0.15603319999999998
-3.74161971	2.91793019	2.973513

-3.65061971	4.7363181800000005	5.4804007
-3.56061971	5.52389144	4.163359
-3.47061971	5.49640636	2.9754446999999997
-3.38061971	3.9096942199999996	1.8212062
-3.28961971	5.6689621	0.7987510000000001
-3.19961971	5.45346564	0.5099256
-3.10961971	4.9763272	0.3826153
-3.01861971	1.69289023	0.0513063
-2.92861971	0.5322654600000001	0.0032483
-2.83861971	0.44585361999999995	0.0016811599999999997
-2.74861971	1.18047274	0.06983107999999999
-2.65761971	6.181937400000001	0.5377514999999999
-2.56761971	5.62942493	0.47553100000000004
-2.47761971	6.07861415	0.4151539
-2.38761971	6.624184769999999	0.5157309
-2.29661971	6.31003304	0.530678
-2.20661971	3.4137679199999997	0.269566
-2.11661971	1.81427224	0.11047459
-2.02661971	2.87643393	0.14929572
-1.93561971	5.63596884	0.27003969000000005
-1.84561971	6.373172210000001	0.22707143000000002
-1.75561971	4.42116363	0.11941849
-1.66561971	0.8157560499999998	0.013201760000000002
-1.57461971	0.15619147	0.00025778
-1.48461971	0.09666343999999999	0.00022178
-1.39461971	0.09776051000000001	0.0004966399999999999
-1.30461971	0.06821496	9.663e-05

-1.21361971	0.057689019999999994	4.677e-05
-1.12361971	0.13961220000000002	0.0005844299999999999
-1.03361971	7.363031400000002	0.03307149
-0.94361971	13.47990977	0.062327900000000006
-0.85261971	13.43941714	0.0880234
-0.76261971	1.36448214	0.0090024
-0.67261971	7.44345654	0.07741750000000001
-0.58261971	10.35795934	0.11499820000000001
-0.49161971	11.77232313	0.300983
-0.40161971	13.535104399999998	1.351006
-0.31161971	7.676315499999999	1.153715
-0.22161971	0.58504561	0.26971639
-0.13061971	5.62224102	9.8717457
-0.04061971	8.14761114	13.584925400000001
0.04938029	0.30685026	0.3862521
0.14038029	0.051732499999999994	0.00021294
0.23038029	0.26775944	0.00091796
0.32038029	0.32117869	0.00217702
0.41038029	0.19750894000000002	0.00196777
0.50138029	0.02997893	0.00022446000000000003
0.59138029	0.04749395	2.923e-05
0.68138029	0.01263061	9.81e-06
0.77138029	0.04542582000000001	5.053e-05
0.86238029	0.05541354	0.00014406
0.95238029	0.35281993	0.00088809
1.04238029	0.41893747000000003	0.0003215699999999997
1.13238029	0.17162384	0.00032201

1.22338029	0.06280431	0.00017282999999999998
1.31338029	0.11360009999999998	7.11e-06
1.40338029	0.44594478000000004	7.252e-05
1.49338029	0.4001721200000001	0.00015741
1.58438029	0.13183558999999997	3.435e-05
1.67438029	0.22082469999999996	0.00023207000000000002
1.76438029	0.226102	0.00038495
1.85438029	0.0762584	5.8639999999999994e-05
1.94538029	0.06622958999999999	5.9980000000000005e-05
2.03538029	0.09532562	7.264999999999999e-05
2.12538029	0.5662973499999999	2.5830000000000002e-05
2.21538029	0.26144148	8.809999999999999e-06
2.30638029	0.0037397099999999994	2.1400000000000003e-06
2.39638029	0.14204537	0.0001906
2.48638029	0.17265351999999998	0.00020243999999999997
2.57638029	0.08407	2.5180000000000003e-05
2.66738029	0.71136795	6.97e-05
2.75738029	1.14871563	0.00048587
2.84738029	0.39793261999999996	0.00030512
2.93738029	0.16368189000000002	3.2460000000000004e-05
3.02838029	0.008376269999999998	1.86e-06
3.11838029	2.46e-06	0.0
3.20838029	0.0	0.0
3.29938029	0.0	0.0
3.38938029	0.0	0.0
3.47938029	0.00035345	2.1999999999999998e-07
3.56938029	0.14204188999999998	7.211e-05

3.66038029	0.7834603899999999	0.0008571000000000001
3.75038029	0.27259807999999996	0.00070552
3.84038029	0.0036664599999999994	1.1860000000000002e-05
3.93038029	3.191e-05	1e-07
4.02138029	0.03638311	0.00010540999999999998
4.11138029	0.4527117400000001	0.00069759
4.20138029	0.70909453	0.00019559
4.29138029	0.29181273	0.0001167
4.38238029	0.3218756300000001	7.296e-05
4.47238029	0.04318198000000001	1.0799999999999998e-05
4.56238029	0.26201224999999995	0.00011698000000000001
4.65238029	0.48551055	0.00402178
4.74338029	0.6708458800000001	0.01955729
4.83338029	0.39874451	0.0031233700000000003
4.92338029	0.7951879199999999	0.07215028000000001
5.01338029	0.69620584	0.09176820000000001
5.10438029	0.20428553000000002	0.0016818700000000002
5.19438029	0.55469431	0.0009807400000000001
5.28438029	0.19289028000000005	0.00247909
5.37438029	0.69387334	0.11524780000000001
5.46538029	0.69797173	0.08288072
5.55538029	0.5222910599999999	0.00543357
5.64538029	0.7968475199999999	0.00042766999999999995
5.73538029	0.17559276999999998	7.483e-05
5.82638029	0.20337115999999994	9.233e-05
5.91638029	0.5756663	0.0010273
6.00638029	0.5760088900000002	0.00121013

6.09638029	0.026138770000000006	5.667e-05
6.18738029	6.3e-06	0.0

Panel (c)

$E - E_F$ / eV	H_2O *sp* pDOS / eV^{-1}	OH^- *sp* pDOS / eV^{-1}
-9.983375	1.8799999999999998e-06	0.0
-9.892375	0.007815560000000001	1e-08
-9.800375	0.11900298000000001	2.5e-07
-9.709375	0.028342779999999998	5e-08
-9.618375	0.36785070999999997	8.8e-07
-9.527375	0.57331231	1.3600000000000001e-06
-9.435375	0.01035132	3.0000000000000004e-08
-9.344375	2.39e-06	0.0
-9.253375	0.020892870000000008	5e-08
-9.162375	0.70279066	2.11e-06
-9.070375	0.33928941999999995	1.0900000000000002e-06
-8.979375	0.53065348	2.2499999999999996e-06
-8.888375	0.48440786	7.1e-07
-8.797375	0.02173695	1e-08
-8.706375	5.21e-06	0.0
-8.614375	1.518e-05	0.0
-8.523375	0.058043040000000004	3e-07
-8.432375	1.1999558099999996	5.11e-06
-8.341375	1.1222926000000002	2.18e-06
-8.249375	0.08840406999999999	2.3000000000000002e-07
-8.158375	0.9559890600000001	3.5199999999999998e-06
-8.067375	0.33105056	1.2200000000000002e-06

-7.976375	0.16898180000000002	1.15e-06
-7.885375	0.06724888000000001	4.4e-07
-7.793375	0.7962695400000002	1.3399999999999999e-06
-7.702375	2.18562455	4.8e-06
-7.611375	2.9736090199999996	1.149e-05
-7.520375	2.5641102600000005	6.6799999999999996e-06
-7.428375	4.0887554800000006	6.22e-06
-7.337375	1.2980578200000001	4.09e-06
-7.246375	0.919651	3.56e-06
-7.155375	4.02391115	1.0660000000000001e-05
-7.063375	2.9856708899999997	5.15e-06
-6.972375	0.32801185	1.9799999999999997e-06
-6.881375	2.5619465999999997	0.0016584
-6.790375	21.530788979999997	0.051742100000000006
-6.699375	24.38908767	0.061441499999999996
-6.607375	1.9557828400000001	0.0085797
-6.516375	13.90190371	0.377531
-6.425375	26.06864146	0.672598
-6.334375	2.3930105	0.056388299999999995
-6.242375	0.30927233	5.3769999999999995e-05
-6.151375	0.04742261000000001	2.9400000000000002e-06
-6.060375	0.20092462	0.01329984
-5.969375	11.22591852	0.7842510100000002
-5.877375	8.56349965	0.5947284100000001
-5.786375	0.12188460999999998	0.0048009
-5.695375	0.11379739999999999	5.0800000000000005e-06
-5.604375	0.14250412000000007	4.68e-06

-5.513375	0.08228989	1.94e-06
-5.421375	0.24590075000000006	4.69e-06
-5.330375	0.17061707999999995	3.13e-06
-5.239375	0.23012147	7.440000000000001e-06
-5.148375	0.26933237000000004	7.500000000000001e-06
-5.056375	0.12664062	6.6799999999999996e-06
-4.965375	0.26056872000000003	1.008e-05
-4.874375	0.36508805000000005	1.976e-05
-4.783375	0.31823958	2.3049999999999998e-05
-4.691375	0.21285658000000002	1.971e-05
-4.600375	0.58173706	4.1809999999999994e-05
-4.509375	0.9955563000000001	0.00012448
-4.418375	0.59031473	0.00017169
-4.327375	0.566784	0.00034059
-4.235375	0.25843307	0.00022542
-4.144375	0.05781234999999999	0.00041152000000000007
-4.053375	0.8662213999999999	0.18554901000000001
-3.962375	9.12993224	1.410922
-3.870375	6.42219356	0.5339657
-3.779375	1.5536182199999997	0.6472912000000001
-3.688375	4.39119681	3.6555748
-3.597375	6.800980999999999	6.479213
-3.505375	4.59741745	3.3259385999999997
-3.414375	5.11383246	2.0740589
-3.323375	1.14330932	0.1661048
-3.232375	0.2890724	0.0026076299999999997
-3.141375	0.23555940000000003	0.00250444

-3.049375	1.0061662999999998	0.043598120000000004
-2.958375	5.737848499999999	0.4271058
-2.867375	6.0570191399999995	0.44423429999999997
-2.776375	6.47842757	0.4217883
-2.684375	5.27928495	0.3964817
-2.593375	5.69546358	0.48243410000000003
-2.502375	5.051743800000001	0.4160413
-2.411375	2.783884	0.18963679999999997
-2.319375	4.392409089999999	0.20008881
-2.228375	5.327949640000001	0.22907964
-2.137375	6.3730988	0.20798689999999997
-2.046375	2.9821043	0.07748377
-1.955375	0.448954	0.00593136
-1.863375	0.23531268	0.0005382200000000001
-1.772375	0.18125238	0.00041197999999999994
-1.681375	0.14054411000000006	0.00025285
-1.590375	0.14837530999999998	0.00010742
-1.498375	0.16882841	0.00045993
-1.407375	7.972442599999999	0.018473490000000002
-1.316375	11.00545709	0.027176729999999996
-1.225375	13.312017139999998	0.06993769999999999
-1.133375	2.64230291	0.01499594
-1.042375	1.0466833199999999	0.00758
-0.951375	13.2449285	0.1066749
-0.860375	6.979745800000001	0.058434900000000005
-0.769375	13.3966674	0.1194955
-0.677375	3.2828643700000004	0.14538089999999998

-0.586375	12.696895990000002	0.7403800000000001
-0.495375	1.5858937899999996	0.0922544
-0.404375	0.22294686	0.011986430000000001
-0.312375	0.30713267000000005	0.03195327
-0.221375	0.97149409	1.99296084
-0.130375	7.7543755700000006	18.3318365
-0.039375	2.70636422	5.790814
0.051625	0.07408786	0.02961526
0.143625	0.08338828	0.00015431
0.234625	0.30852069	0.00193379
0.325625	0.34457768	0.00297189
0.416625	0.07496618000000002	0.0009564700000000001
0.508625	0.019402649999999997	1.54e-05
0.599625	0.0373271	2.209e-05
0.690625	0.019330100000000003	1.997e-05
0.781625	0.04391836	8.554999999999999e-05
0.873625	0.20920984000000006	0.0009564400000000001
0.964625	0.31280736000000003	0.00062255
1.055625	0.37501182	0.00036158
1.146625	0.10118176999999999	0.00033371000000000003
1.237625	0.011591309999999999	5.989999999999999e-06
1.329625	0.31740406000000004	0.00012166999999999999
1.420625	0.42469734000000003	0.00015835
1.511625	0.2928583199999999	4.870999999999999e-05
1.602625	0.19949550000000002	0.0002434
1.694625	0.24052325	0.0005126099999999999
1.785625	0.07937282	0.00010428

1.876625	0.06666458000000001	6.81e-05
1.967625	0.06362751	9.405e-05
2.059625	0.27040265	2.199e-05
2.150625	0.5475121900000001	2.311e-05
2.241625	0.03934905000000001	2.7479999999999998e-05
2.332625	0.12027080999999999	0.00038503
2.423625	0.13625325999999996	0.00010450999999999999
2.515625	0.08402693	2.536e-05
2.606625	0.47548682999999997	0.00014077000000000002
2.697625	1.30465039	0.0007779899999999999
2.788625	0.4464383900000001	0.00018395
2.880625	0.16598549	3.623e-05
2.971625	0.008406930000000002	2.47e-06
3.062625	8.53e-06	2e-08
3.153625	0.0	0.0
3.245625	0.0	0.0
3.336625	5e-08	0.0
3.427625	0.0018737799999999998	5.7999999999999995e-06
3.518625	0.23378415	0.00067139
3.609625	0.77186248	0.00132042
3.701625	0.14610868999999999	0.00017155
3.792625	0.0006784	8.100000000000001e-07
3.883625	0.007238629999999999	3.34e-05
3.974625	0.17953	0.0008312199999999999
4.066625	0.21952326	0.00031253
4.157625	0.7559833299999997	0.0005518
4.248625	0.33084779999999997	0.00286583

4.339625	0.35809893	0.01689683
4.431625	0.05709956	0.00314147
4.522625	0.68257769	0.0767133
4.613625	0.8598523199999999	0.07864460000000001
4.704625	0.70967261	0.005896170000000001
4.795625	0.45800384	0.00207895
4.887625	0.28963087	0.005357540000000001
4.978625	0.60883189	0.1303679
5.069625	0.67649966	0.07322819
5.160625	0.7133175499999999	0.07727974
5.252625	0.38053403	0.07773714
5.343625	0.30342166	0.02724464
5.434625	0.32079058	0.0034143299999999997
5.525625	0.8465892500000001	0.01599706
5.617625	0.5128847799999999	0.02543886
5.708625	0.58424272	0.1814357
5.799625	0.27210937	0.07079233
5.890625	0.17326870000000003	0.03034141
5.981625	0.006728039999999999	0.00110844
6.073625	1.43e-06	2.5e-07

Panel (d)

$E - E_{\mathrm{F}}$ / eV	H_2O *sp* pDOS / eV^{-1}	OH^- *sp* pDOS / eV^{-1}
-10.79938622	8.383e-05	0.0
-10.69738622	0.05010134	9e-08
-10.59538622	0.08936830000000001	1.6e-07
-10.49438622	0.07754546000000001	1.5e-07

-10.39238622	0.7441558399999999	1.4700000000000001e-06
-10.29038622	0.05725250999999986	1.2000000000000002e-07
-10.18938622	5.18e-06	0.0
-10.08738622	0.0006923500000000001	0.0
-9.98538622	0.35444989000000005	8.8e-07
-9.88438622	0.59185058	1.48e-06
-9.78238622	0.25121085000000004	1.06e-06
-9.68038622	0.62454318	1.29e-06
-9.57938622	0.11176016	5e-08
-9.47738622	8.967e-05	0.0
-9.37538622	4.2e-07	0.0
-9.27438622	0.021078020000000003	8e-08
-9.17238622	1.03486569	3.7099999999999996e-06
-9.07038622	1.1377394499999998	1.7500000000000002e-06
-8.96938622	0.12484693	2.6e-07
-8.86738622	1.0172614099999997	2.85e-06
-8.76638622	0.10387063000000002	2.9e-07
-8.66438622	0.01895567	9.000000000000001e-08
-8.56238622	0.42965732	1.1699999999999998e-06
-8.46138622	2.3744039299999993	3.12e-06
-8.35938622	3.85983128	6.749999999999999e-06
-8.25738622	3.9951627700000003	6.5900000000000004e-06
-8.15638622	1.35693094	3.2599999999999997e-06
-8.05438622	0.19825721	7.7e-07
-7.95238622	2.9356560199999997	5.989999999999999e-06
-7.85138622	3.77477017	5.6e-06
-7.74938622	0.55275595	7.5e-07

-7.64738622	1.6264448000000002	2.88e-06
-7.54638622	2.7471764	2.84e-06
-7.44438622	0.5345803699999998	1.339e-05
-7.34238622	3.7748877999999997	0.018650669999999998
-7.24138622	29.162275320000003	0.1052271
-7.13938622	7.2685148700000015	0.01229333
-7.03738622	10.580519540000003	0.3295325
-6.93638622	24.812118639999998	0.675242
-6.83438622	2.9989143399999993	0.0697107
-6.73338622	0.06950430000000002	2.897e-05
-6.63138622	0.043186680000000005	4.33e-06
-6.52938622	0.47730573	0.02908425
-6.42838622	13.87685001	0.94652459
-6.32638622	3.94582044	0.26337626
-6.22438622	0.19345031	0.00023714
-6.12338622	0.07000939	4.14e-06
-6.02138622	0.10307620999999999	2.95e-06
-5.91938622	0.24085152999999998	5.46e-06
-5.81838622	0.22177022	4.74e-06
-5.71638622	0.10996336000000001	4.14e-06
-5.61438622	0.34125439999999996	1.075e-05
-5.51338622	0.15360206000000004	2.6700000000000003e-06
-5.41138622	0.38373567000000003	1.252e-05
-5.30938622	0.7083858900000001	2.566e-05
-5.20838622	0.7261350799999999	3.8350000000000004e-05
-5.10638622	0.37136739999999996	3.115e-05
-5.00438622	0.4571769699999999	9.931e-05

-4.90338622	0.31938034	0.00014566
-4.80138622	0.07320302999999999	7.405000000000001e-05
-4.70038622	0.02222378	4.1989999999999996e-05
-4.59838622	0.25752133	0.01992282
-4.49638622	8.341154750000001	0.7718169
-4.39538622	7.116671159999999	0.4468525
-4.29338622	1.07629273	0.0807617
-4.19138622	4.48398792	0.7481173999999999
-4.09038622	6.1886547	1.4942901
-3.98838622	3.5924729300000005	5.0325951
-3.88638622	4.3807488	6.2056962
-3.78538622	1.5276199400000001	1.6810307
-3.68338622	0.2751593100000001	0.01828129
-3.58138622	0.27900269000000005	0.00360065
-3.48038622	1.70060018	0.15188359999999998
-3.37838622	6.921092789999999	0.569652
-3.27638622	5.848531889999999	0.445319
-3.17538622	4.8212803399999995	0.3849808
-3.07338622	6.26450938	0.539709
-2.97238622	5.0635747	0.4632155
-2.87038622	2.89281287	0.21582300000000001
-2.76838622	3.0661531500000003	0.13438946000000002
-2.66738622	5.4469382	0.21705107
-2.56538622	6.182115919999999	0.18226489
-2.46338622	3.3944858900000003	0.07638076
-2.36238622	0.4764850899999999	0.00564039999999999
-2.26038622	0.10402584000000002	0.00023941999999999998

-2.15838622	0.18702586000000002	0.00030732000000000003
-2.05738622	0.14735672000000005	0.00040564999999999997
-1.95538622	0.053420709999999996	0.00027952
-1.85338622	5.6216792799999995	0.011294619999999998
-1.75238622	22.35058006	0.0801507
-1.65038622	3.7200029899999993	0.02047902
-1.54838622	0.7578989700000001	0.00485115
-1.44738622	13.06273323	0.098285
-1.34538622	7.25343916	0.0515167
-1.24338622	10.844642310000001	0.0759499
-1.14238622	1.0475553100000001	0.022788720000000002
-1.04038622	12.23298536	0.381633
-0.93938622	2.5706169699999997	0.08015359999999999
-0.83738622	0.09420368000000001	0.0012158499999999999
-0.73538622	0.15623241999999998	0.00229847
-0.63438622	0.17021032	0.00443019
-0.53238622	0.17700304	0.03182806
-0.43038622	2.0557312000000003	5.91825231
-0.32938622	6.44554546	15.976628599999998
-0.22738622	1.2169452	2.39373427
-0.12538622	0.08047987	0.00240757
-0.02438622	0.05469320999999999	0.00016814
0.07761378	0.007820609999999999	4.599999999999999e-06
0.17961378	0.06698579	2.142e-05
0.28061378	0.19040932000000005	0.00020674
0.38261378	0.28243562000000005	0.00062573
0.48461378	0.17178538999999998	0.00012122

0.58561378	0.1359159	0.00035955000000000004
0.68761378	0.04381577999999999	0.00025107
0.78961378	0.00567265	2.0799999999999996e-06
0.89061378	0.045086960000000016	7.4700000000000005e-06
0.99261378	0.0076445	1.88e-06
1.09361378	0.06541405	2.758e-05
1.19561378	0.23249676000000002	0.00017587
1.29761378	0.5070681999999999	0.00040297
1.39861378	0.13150115	0.00013125
1.50061378	0.06038556999999999	9.041000000000001e-05
1.60261378	0.11440099999999997	0.00017067999999999999
1.70361378	0.16079158999999998	8.380000000000001e-06
1.80561378	0.46312796999999994	3.147e-05
1.90761378	0.31129126	9.596e-05
2.00861378	0.01644166	1.581e-05
2.11061378	0.021582909999999997	1.443e-05
2.21261378	0.21661858999999997	0.00014699
2.31361378	0.21815779000000002	0.00024066999999999998
2.41561378	0.05857681	3.7879999999999996e-05
2.51761378	0.44972473999999996	3.456e-05
2.61861378	0.4215428799999999	6.193e-05
2.72061378	0.03437467999999999	1.8069999999999998e-05
2.82261378	0.010492930000000001	1.11e-06
2.92361378	0.17177884	0.00010588000000000001
3.02561378	0.14390113000000004	0.00014485000000000002
3.12661378	0.04480958	1.386e-05
3.22861378	0.28444639	5.74e-06

3.33061378	0.85120971	0.00012924
3.43161378	0.57490832	0.0003186599999999996
3.53361378	0.37456964000000004	0.00014067
3.63561378	0.15320592000000005	2.367e-05
3.73661378	0.0036702	4.9e-07
3.83861378	6.999999999999999e-08	0.0
3.94061378	0.0	0.0
4.04161378	0.0	0.0
4.14361378	1.6130000000000007e-05	0.0
4.24561378	0.03950213	2.874e-05
4.34661378	0.3862277200000001	0.00057569
4.44861378	0.49844718000000005	0.00051474
4.55061378	0.07503995999999999	5.94e-06
4.65161378	7.026000000000001e-05	0.0
4.75361378	0.01022677	2.976e-05
4.85561378	0.18176344000000003	0.0005290500000000001
4.95661378	0.15850698000000005	8.683000000000001e-05
5.05861378	0.6679246	6.743e-05
5.15961378	0.19404590000000002	3.557e-05
5.26161378	0.15211664	9.225999999999999e-05
5.36361378	0.16976246	0.00012893
5.46461378	0.08231413999999998	9.507e-05
5.56661378	0.46569051	0.00909662
5.66861378	0.7175114699999998	0.00893108
5.76961378	0.7659472099999999	0.02924069
5.87161378	0.68123073	0.08408347000000001
5.97361378	0.05339762	0.0030093399999999997

6.07461378	0.22985909000000002	0.00023972000000000002
6.17661378	0.5034270500000001	0.00985711
6.27861378	0.52571727	0.11294099999999999
6.37961378	0.16056971	0.011120429999999999
6.48161378	0.29061652	0.00105298
6.58361378	0.8059964899999998	0.00159728
6.68461378	0.46439013	0.00024559
6.78661378	0.01560605	1.775e-05
6.88861378	0.58412004	0.0008135600000000001
6.98961378	0.57457389	0.00087429
7.09161378	0.011788000000000002	1.916e-05
7.19261378	3.0000000000000004e-07	0.0

Figure 3

Panel (a)

Disp. / Å	$q_{\sigma=0.0}$, GGA	$q_{\sigma=0.0}$, hybrid	$q_{\sigma=-0.75}$, GGA
0.0	0.73	0.768	0.67
0.5	0.8566	0.8823	0.804
1.1	0.9655	0.9758	0.937
1.6	0.9887	0.9914	0.9801
2.1	0.9936	0.9949	0.989
2.7	0.9978	0.9981	0.9952
3.2	0.9995	0.9991	0.9977
3.7	0.9995	0.9995	0.9986
4.3	1.0001	0.9999	0.9993
4.8	1.0001	1.0001	0.9997

5.3	1.0003	0.9999	0.9954
5.9	0.9999	0.9999	0.9999
6.4	0.9999	1.0001	0.9995
6.9	1.0	0.9999	0.9999
7.5	0.9999	1.0001	0.9953
8.0	1.0001	1.0	0.9951

Panel (b)

Disp. / Å	$q_{\sigma=0.0}$, GGA	$q_{\sigma=0.0}$, hybrid	$q_{\sigma=-0.75}$, GGA
0.0	-0.6655	-0.8052	-0.7923
0.5	-0.7483	-0.9097	-0.8926
1.1	-0.781	-0.9734	-0.9563
1.6	-0.7522	-0.9929	-0.9846
2.1	-0.8063	-0.9977	-0.9896
2.7	-0.7564	-0.9993	-0.9968
3.2	-0.7229	-0.9997	-0.9891
3.7	-0.7869	-0.9998	-0.9952
4.3	-0.8116	-0.9999	-0.9916
4.8	-0.8062	-1.0	-0.9942
5.3	-0.7808	-0.9999	-0.9939
5.9	-0.7994	-1.0	-0.992
6.4	-0.7705	-0.9999	-0.9963
6.9	-0.718	-1.0001	-0.9963
7.5	-0.7927	-1.0001	-0.9965
8.0	-0.806	-0.9999	-0.9906

Figure 4

$\overline{\Phi}$ / eV	$\Delta E_{\mathrm{Volmer}}$ / eV
3.4921975894	0.41228115
3.31276345216	0.05828362
3.50124449053	0.40755005
3.97213329569	0.56833331
4.92543676045	1.15583637
4.23253501559	0.69921263
4.84212512552	1.17792458
4.46869713414	1.27473009
4.60489051465	1.20431931