Supporting Information for "Effects of applied voltage on water at a gold electrode interface from *ab initio* molecular dynamics"

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Contents

1 Additional electrostatic data

The computed electrode potentials for each trajectory presented in the main text follow from the solution and metal potentials Φ_S and Φ_M, respectively. The values of these quantities at every ∼48 fs for each trajectory are given in Figs. S1 and S2. As is mentioned in the main text and is visible here, Φ_M was the more volatile quantity of these two and contributed to most of the magnitude of the fluctuations in Φ_e.

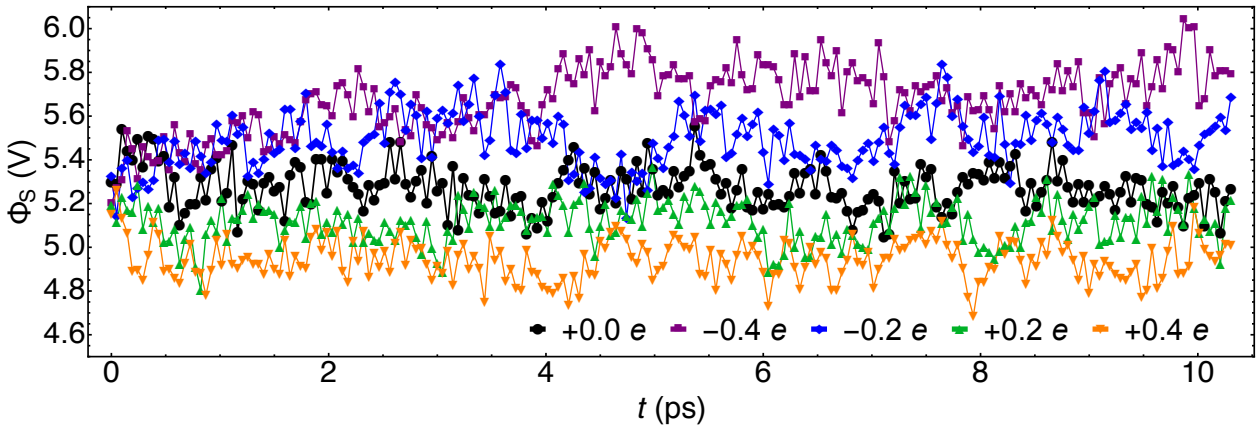

Figure S1: Solution potentials Φ_S as a function of simulation time t for each trajectory, designated by their electrode charges σ.

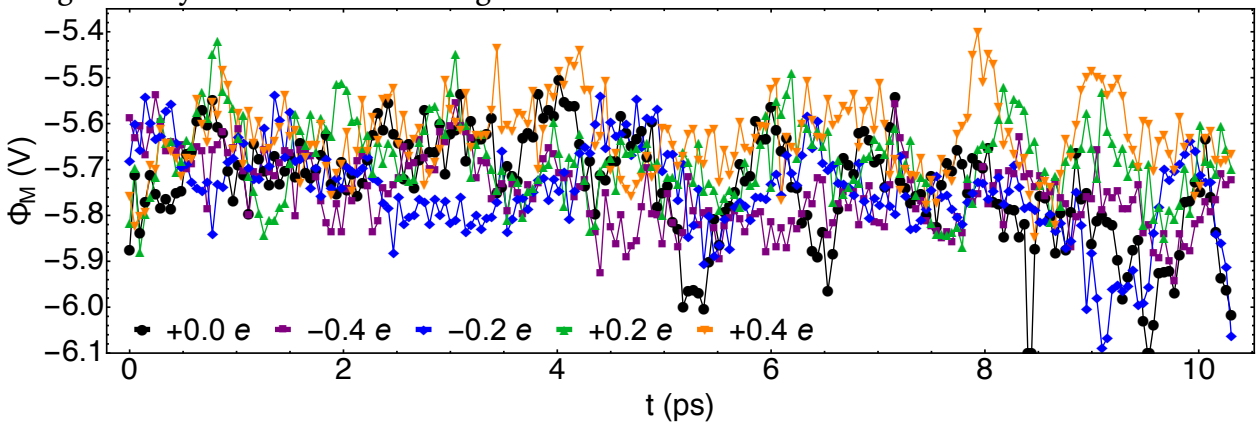

Figure S2: Metal potentials Φ_M as a function of simulation time t for each trajectory, designated by their electrode charges σ.

We chose to measure Φ_M as the value of $\bar{\bar{\Phi}}$ in the back 1 Å of the Au(111) slab because of the stability of this quantity relative to alternatives. To illustrate this, we plotted the value of Φ_M throughout the $\sigma = +0.2\ e$ trajectory as measured three different ways in

Fig. S3. The relative behaviors of Φ_M measured each way were similar for each trajectory. These values demonstrate that the method utilized for the data in Fig. S2 and in the main text avoided the very large fluctuations likely associated with the sampling of unusual, or far from equilibrium atomic structures during the dynamics. We can further rationalize this choice by the limitation of relatively short trajectories and our interest in water under bias at thermal equilibrium. The fluctuations of Φ_M even with our chosen method were large compared to those of Φ_S, underscoring the trade-off between fluctuations in potential vs. charge in fixed-charge and fixed-potential methodologies, respectively.

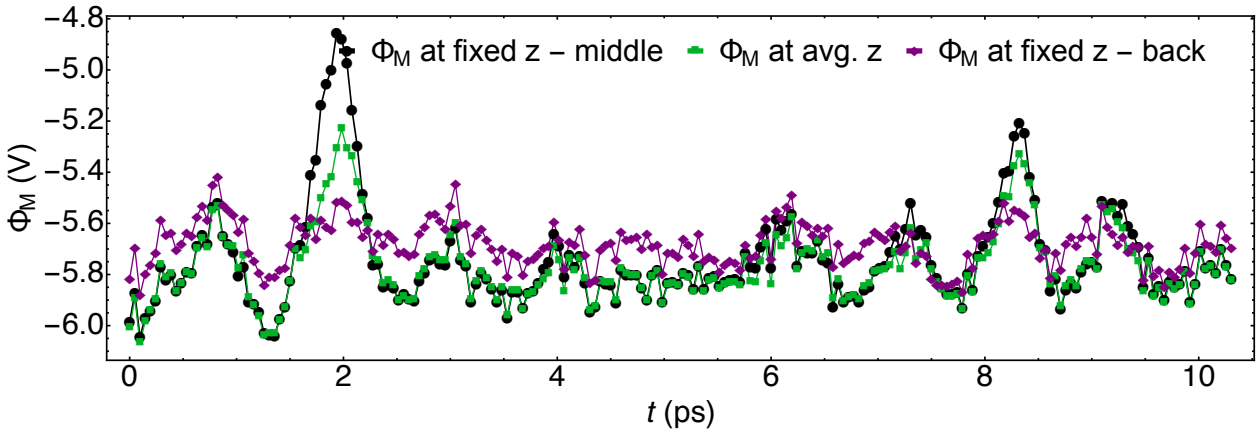

Figure S3: Values of Φ_M for the $\sigma = +0.2\ e$ trajectory as computed as the value of $\bar{\bar{\Phi}}$ at a fixed z near the middle of the slab (black), the value of $\bar{\bar{\Phi}}$ at the average value of z for all Au atoms (green), and as the average value of $\bar{\bar{\Phi}}$ in the back 1 Å of the Au slab, within the fixed layer (purple; same as corresponding data in Fig. S2).

The system's Fermi level E_F exhibits even larger fluctuations than Φ_M, measured any way, during the trajectories, as shown in Fig. S4. While the system's Fermi energy has been used as a reliable metal potential in static or other applications,[1–4] it was satisfactory in this work to utilize the more stable Φ_M as measured at the partially-frozen back of the Au(111) slab.

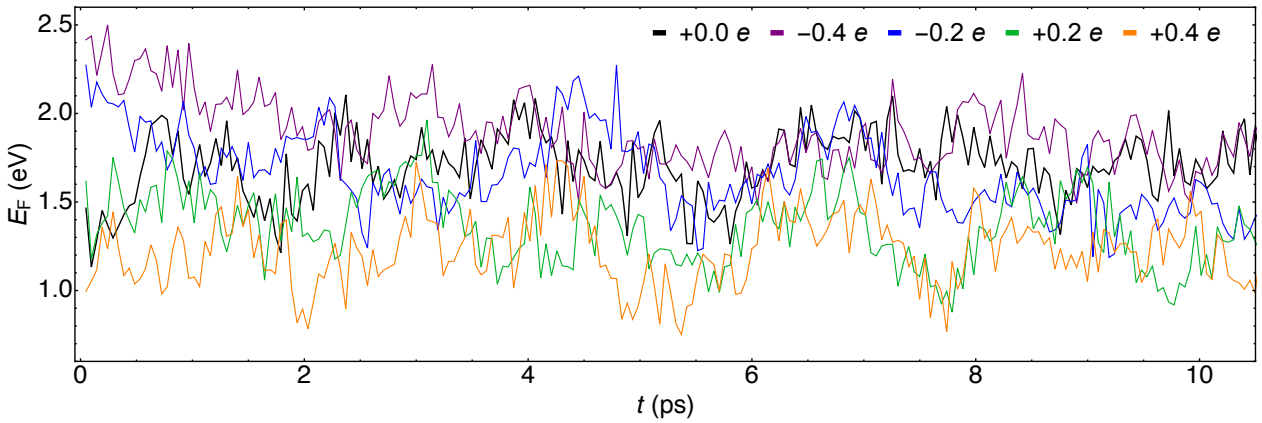

Figure S4: Computed Fermi energies E_F of the system every 100 MD steps (∼0.48 fs) in each trajectory. Note that the scale on which this quantity is plotted is much larger than that of Φ_M in Fig. S2.

2 Water hydrogen bonding and orientations

The structural properties of water at the Au(111) interface were further quantified by counting the average numbers of hydrogen bonds formed by water as functions of both its layer and the applied voltage vs. PZC, φ. Hydrogen bonds were defined by O atoms being less than 3.5 Å apart with an ODO angle within 30° of colinear.[5] The average numbers of hydrogen bonds formed by water molecules in each layer were further distinguished by whether the hydrogen bond was formed with another water molecule of the same or of a neighboring layer. These values are reflected in Figs. S5-S7.

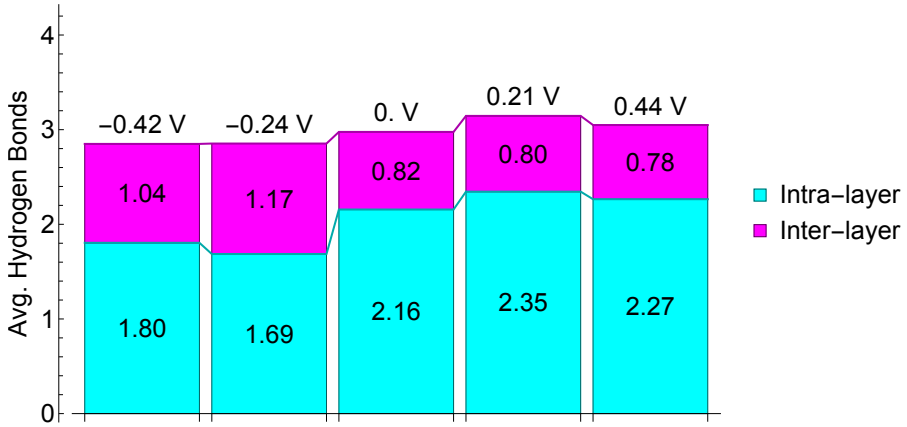

Figure S5: Average numbers of hydrogen bonds in layer 1 of water as a function of φ, delineated by intra- (cyan) and inter-layer (magenta) contributions. Layer 1 water formed fewer hydrogen bonds than water in layers 2 and 3. Water in this layer formed more hydrogen bonds at $\varphi \geq 0$ V vs. PZC and the proportion of intra-layer hydrogen bonds generally increased with φ.

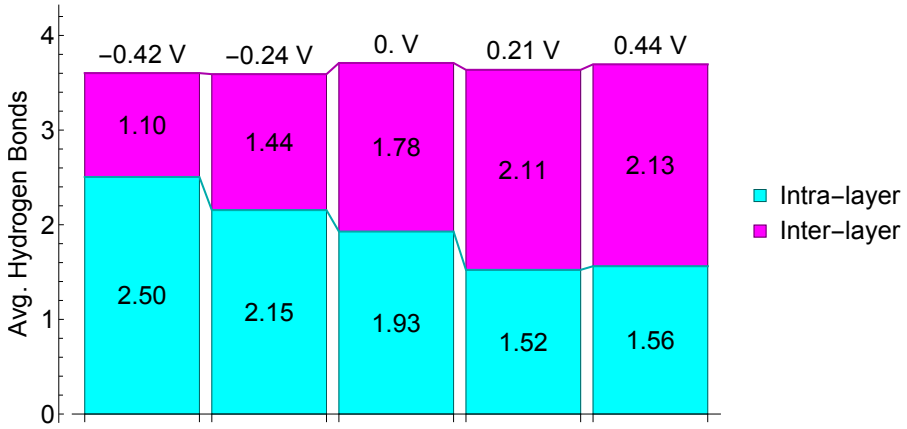

Figure S6: Average numbers of hydrogen bonds in layer 2 of water as a function of φ, delineated by intra- (cyan) and inter-layer (magenta) contributions. Water in layer 2 demonstrated the most overall hydrogen bonds of the three layers studied. The overall number of hydrogen bonds in this layer was not apparently φ-dependent, although the proportion of intra-layer hydrogen bonds generally decreased with φ, in opposition to the trend in layer 1.

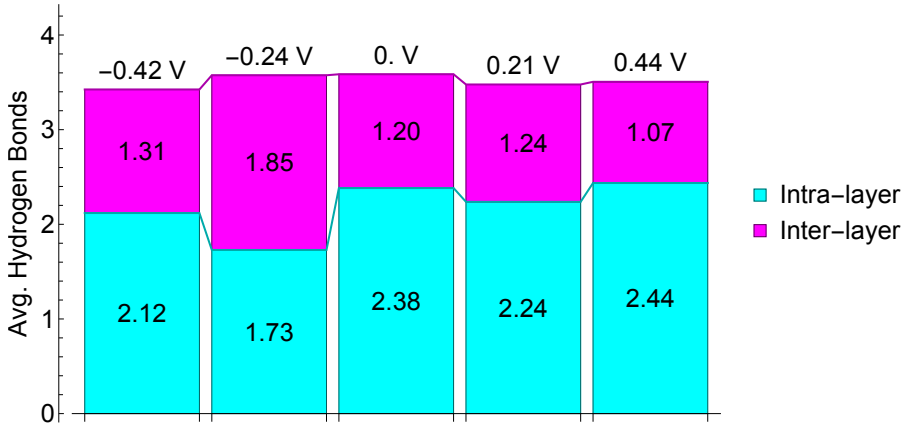

Figure S7: Average numbers of hydrogen bonds in layer 3 of water as a function of φ, delineated by intra- (cyan) and inter-layer (magenta) contributions. Layer 3 water formed slightly fewer hydrogen bonds on average compared to layer 2, and neither the overall number nor the proportion of intra- to inter-layer hydrogen bonds demonstrated a clear dependence on φ.

From Fig. S5 it is evident that the total average number of hydrogen bonds formed by layer 1 water is lower at negative φ than at PZC and positive φ. Additionally in layer 1, we observed an increase in the number intra-layer hydrogen bonding and a decrease in inter-layer hydrogen bonding when going from negative φ to zero and positive φ. That layer 1 water at $\varphi \geq 0$ V exhibits more overall and intra-layer hydrogen bonds than at $\varphi < 0$ is consistent with the higher densities observed at these potentials. This observation is likely also a consequence of the O atom being more likely than not oriented towards the Au surface at non-negative φ given that the O atom typically participates in two hydrogen bonds compared to one for H atoms. Therefore, when O is oriented towards Au and not towards layer 2, its ability to form *inter-layer* hydrogen bonds is suppressed. The hydrogen bonding similarities between the system at PZC and at $\varphi > 0$ in layer 1 are consistent with their similarities in density as a function of z as well.

Figs. S6 and S7 demonstrate that layer 2 water participates in the most hydrogen bonds overall of the 3 studied. The average overall numbers of hydrogen bonds formed per water in layers 2 and 3 did not show any clear dependence on φ, consistent with the diminished dependence of $D_{\|}$ and the VDOS spectra on φ in these two layers. In addition, the proportion of intra- and inter-layer hydrogen bonds in layer 2 with respect to φ was

opposite to that in layer 1. In layer 3, the hydrogen bonding data did not seem to depend on φ and the differences with φ were likely within the error of the short simulations.

The effects of φ on water's orientation persisted beyond layer 1, the data for which is given in the main text. The orientations of the water bisectors and OD bonds with respect to surface normal for all layers and φ are given in Figs. S8 and S9.

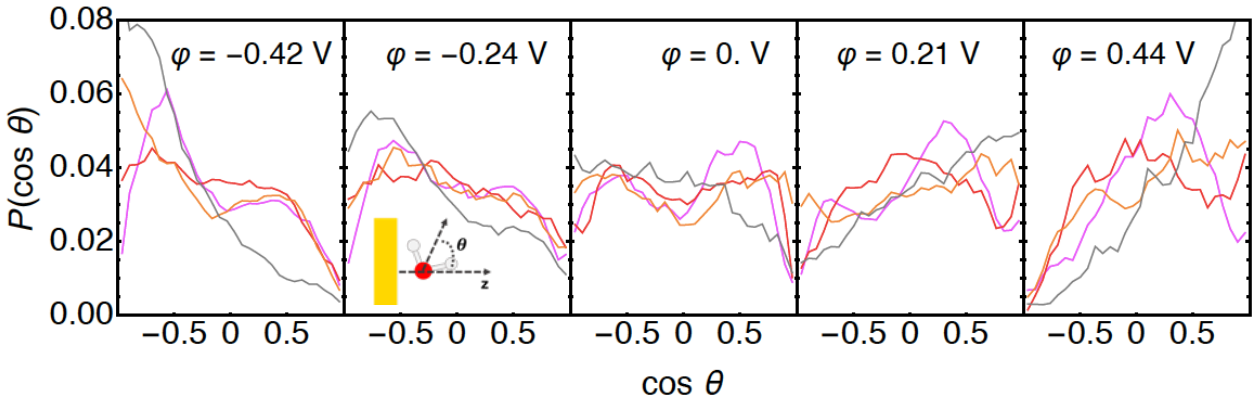

Figure S8: Histograms of the cosines of the angles formed between water's bisector and a unit vector in z for all φ and all layers (1: magenta, 2: red, 3: orange, 4: gray). The inset illustration indicates the relevant angle θ in which the yellow rectangle represents the Au slab, the O atom is red, and the D atoms are white. The effects of φ on water's orientations relative to surface-normal were strongest in layer 1, but persisted into layers 2 and 3.

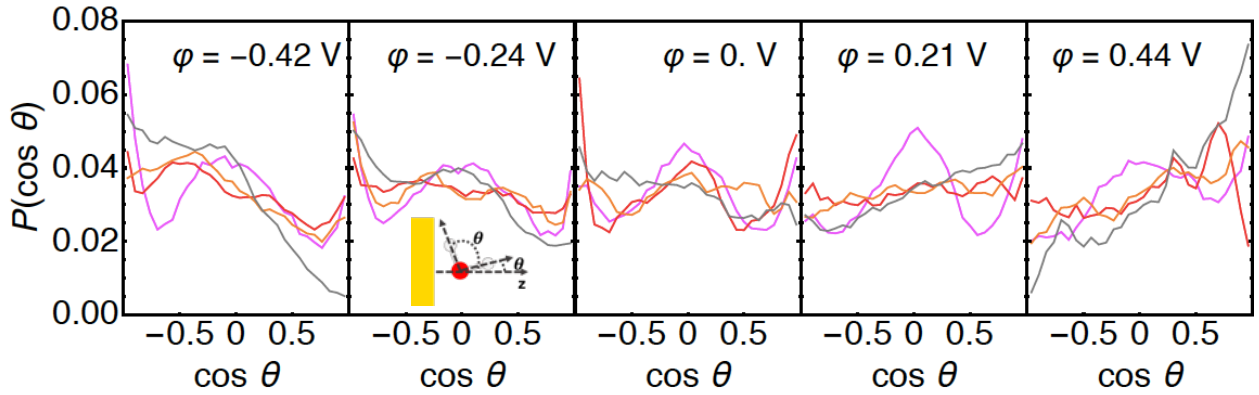

Figure S9: Histograms of the cosines of the angles formed between OD bond vectors and a unit vector in z for all φ and all layers (1: magenta, 2: red, 3: orange, 4: gray). The inset illustration indicates the relevant angles θ in which the yellow rectangle represents the Au slab, the O atom is red, and the D atoms are white. The effects of φ on the orientations of water's OD bonds relative to surface-normal were strongest in layer 1, but persisted into layers 2 and 3.

3 Mean square displacements

The O atom MSDs in x and y up to about half of the total trajectory times for each φ and layers 1-3 were computed to determine the values of $D_{\|}$ shown in the main text. These are depicted here in Figs. S10-S12. The best fit slopes of the xy MSDs were used in Einstein's relation to obtain the 2D diffusion coefficients.

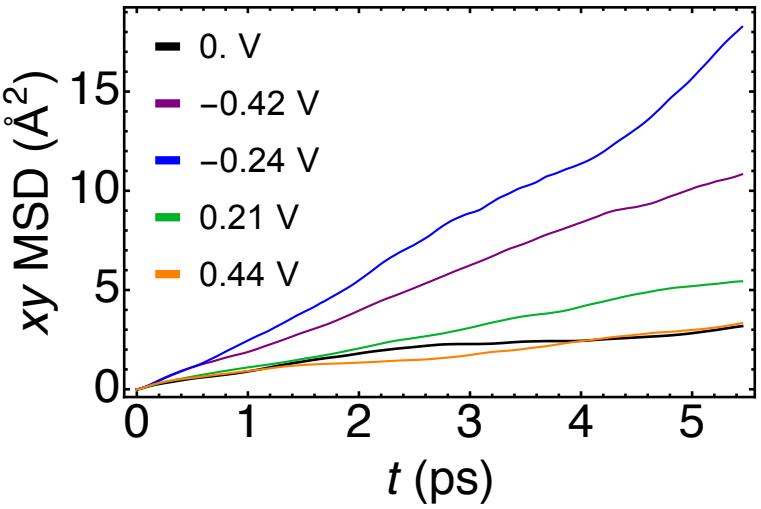

Figure S10: Mean-square displacements in x and y for water O atoms in layer 1 for each φ as a function of simulation time t up to about half of the total BOMD trajectory time. The slopes of the best linear fits to these MSDs were related to the parallel diffusion coefficients $D_{\|}$ shown in the main text. Water in this layer diffused parallel to the surface most at negative φ, consistent with their lower densities and the layer's greater distance from the surface. That the displacements of O atoms in layer 1 were smaller at positive φ is also consistent with the O atom being electrostatically attracted to the surface. Note that deviations from linearity for some trajectories are reflected in the large error bars in Fig. 7.

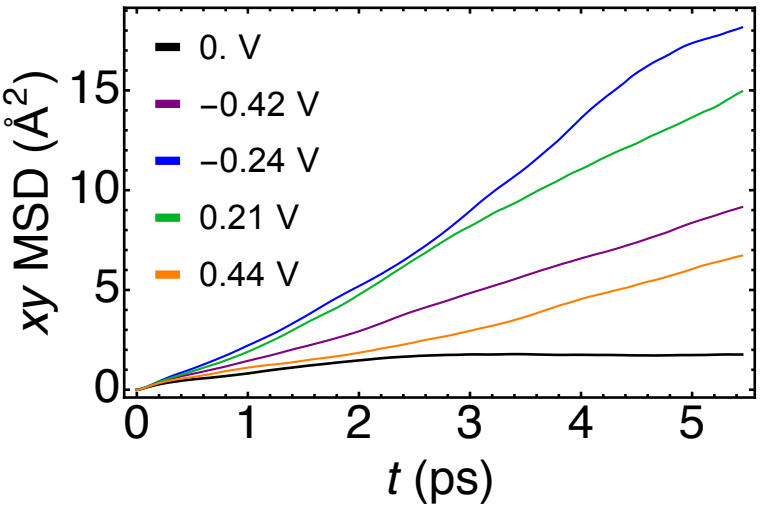

Figure S11: Mean-square displacements in x and y for water O atoms in layer 2 for each φ as a function of simulation time t up to about half of the total BOMD trajectory time. The slopes of the best linear fits to these MSDs were related to the parallel diffusion coefficients $D_{\parallel}$ shown in the main text. Water in layer 2 diffused parallel to the surface most at small, non-zero φ, regardless of sign. At the largest in magnitude values of φ, water diffused parallel to the surface more than at PZC. Note that deviations from linearity for some trajectories are reflected in the large error bars in Fig. 7.

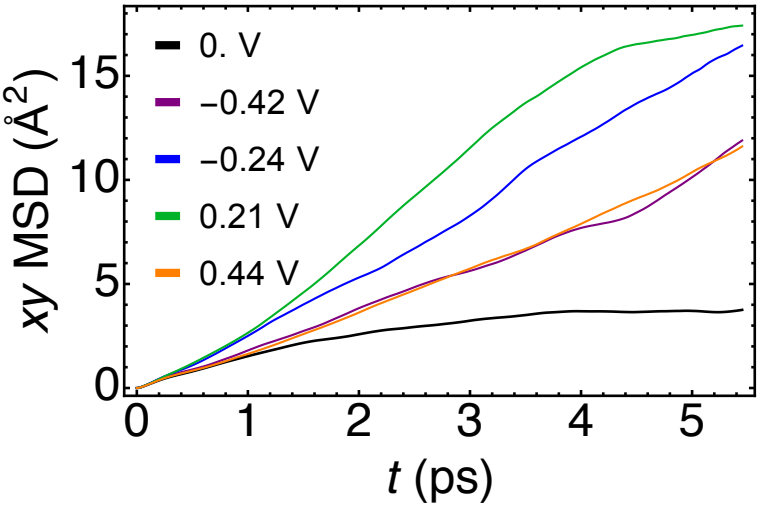

Figure S12: Mean-square displacements in x and y for water O atoms in layer 3 for each φ as a function of simulation time t up to about half of the total BOMD trajectory time. The slopes of the best linear fits to these MSDs were related to the parallel diffusion coefficients $D_{\parallel}$ shown in the main text. Water in layer 3 diffused parallel to the surface most at small, non-zero φ, regardless of sign. At the largest in magnitude values of φ, water diffused parallel to the surface more than at PZC. Note that deviations from linearity for some trajectories are reflected in the large error bars in Fig. 7.

4 Velocity autocorrelation functions

The velocity autocorrelation functions of all water atoms for each φ and layers 1-3 were computed and shown in Figs. S13-S15. The first 1200 fs of each were Fourier transformed to obtain the corresponding VDOS spectra.

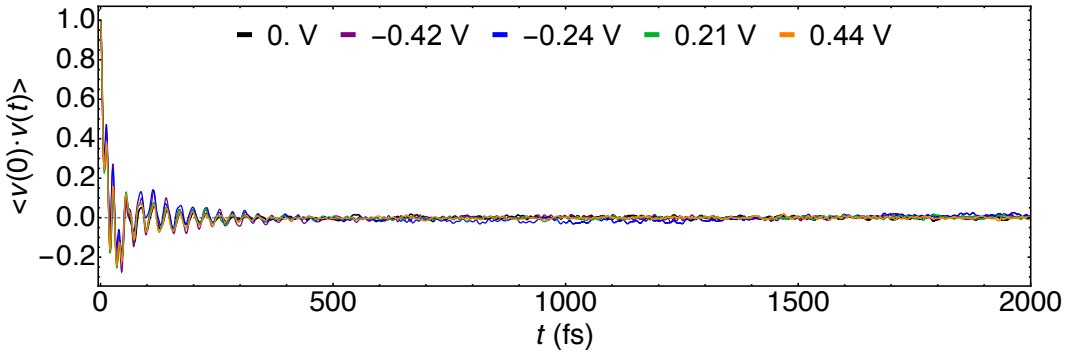

Figure S13: Velocity autocorrelation functions $\langle v(0)v(t)\rangle$ of water O and D atoms in layer 1 for each φ. The first 1200 fs were Fourier transformed to obtained the VDOS spectra shown in the main text.

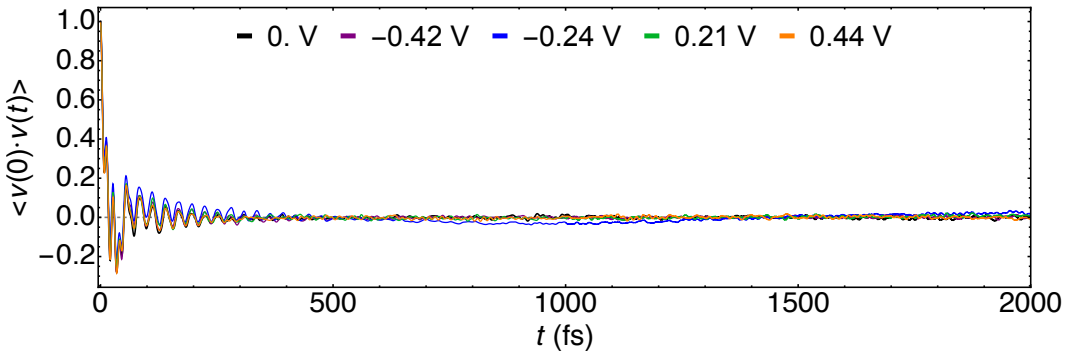

Figure S14: Velocity autocorrelation functions $\langle v(0)v(t)\rangle$ of water O and D atoms in layer 2 for each φ. The first 1200 fs were Fourier transformed to obtained the VDOS spectra shown in the main text.

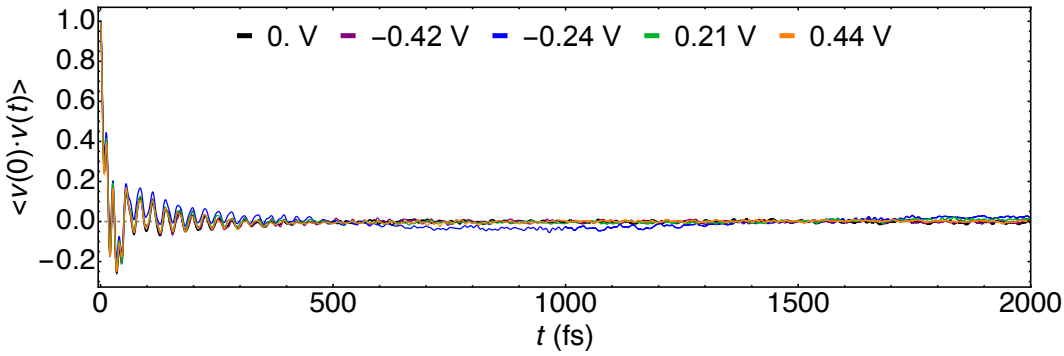

Figure S15: Velocity autocorrelation functions $\langle v(0)v(t)\rangle$ of water O and D atoms in layer 3 for each φ. The first 1200 fs were Fourier transformed to obtained the VDOS spectra shown in the main text.

5 Additional VDOS spectra and analysis

The VDOS spectra shown in the main text were obtained from the Fourier-transformed velocity autocorrelation functions, followed by Gaussian convolution. The resolution of the VDOS spectra that corresponds to the ∼0.48 fs time step was about ∼27 cm^{-1}. We further note here that the interpretations of the VDOS spectra are limited to mainly qualitative observations regarding the effects of distance from the surface and φ given the relatively short BOMD trajectories.

Figs. S16-S18 show the referenced VDOS spectra for layers 1-3 corresponding to those in the main text, with the $\varphi = 0$ V spectrum of each layer as the reference. These referenced spectra are all plotted on the same scale. The referenced spectra highlight shifts and differences in intensity at different φ for each of the first three layers of water from the electrode. These spectra are clearly most intense in layer 1, where the effects of the electrode electrification are greatest. The referenced spectra for layer 1 demonstrate that both the δDOD and νOD peaks are blue shifted at non-zero φ. The referenced νOD signals in layers 2 and 3 for non-zero φ are slightly negative at the lower frequencies characteristic of νOD and slightly positive at the higher frequencies characteristic of νOD. This is consistent of water molecules in layers 2 and 3 being somewhat oriented according to the screened electric field (Figs. S8 and S9).

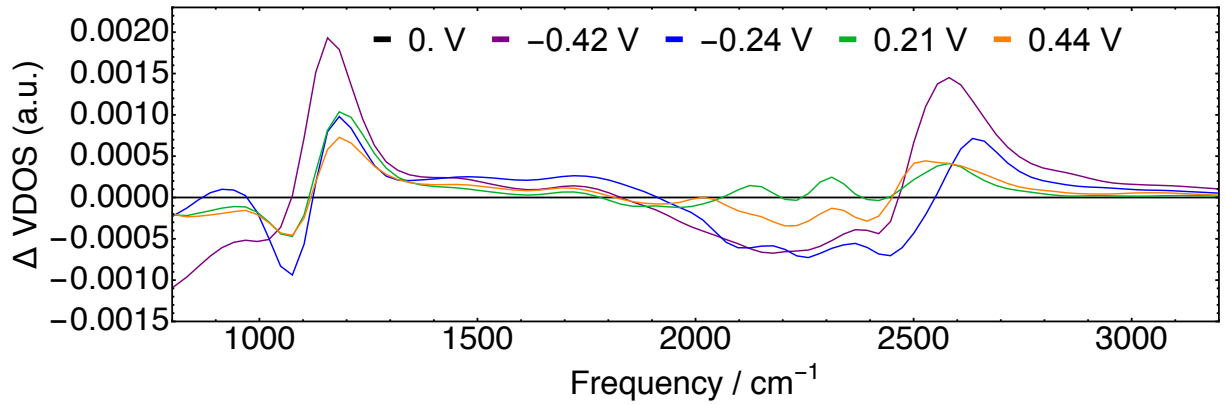

Figure S16: VDOS spectra at each φ for layer 1 water referenced to PZC (black; zero by construction). Negative intensities at lower frequencies and positive intensities at higher frequencies around both regions of interest are representative of blue shifts of both peaks at non-zero φ.

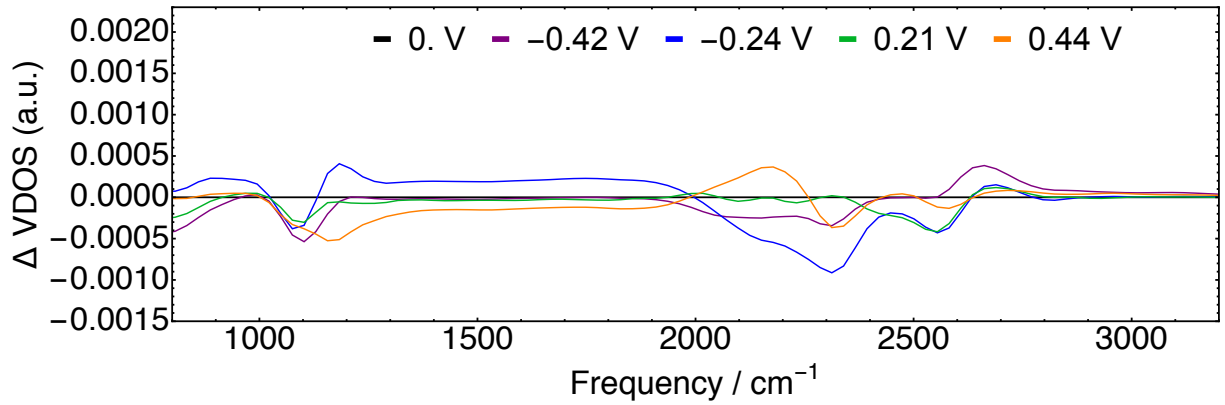

Figure S17: VDOS spectra at each φ for layer 2 water referenced to PZC (black; zero by construction). The lower intensities relative to layer 1 are indicative of a lesser effect of the electrode potential on the vibrational spectra.

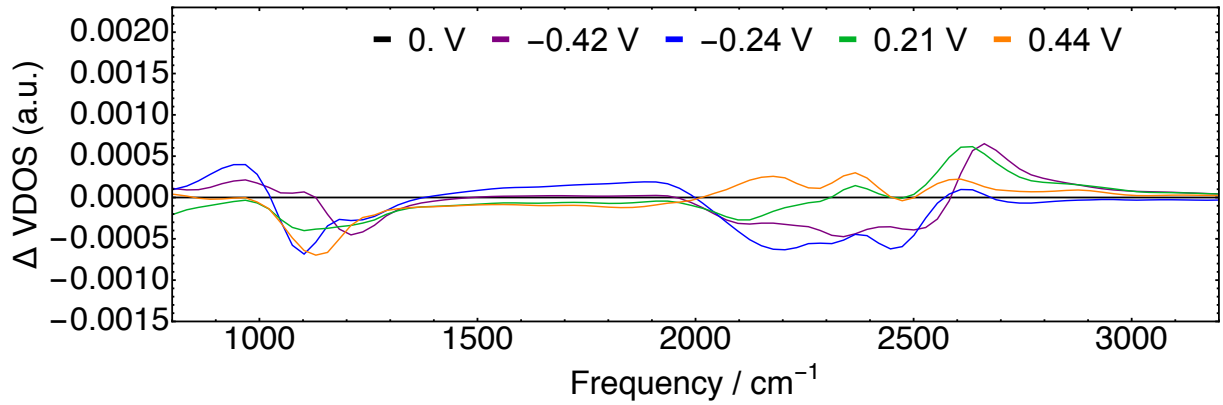

Figure S18: VDOS spectra at each φ for layer 3 water referenced to PZC (black; zero by construction). The lower intensities relative to layer 1 are indicative of a lesser effect of the electrode potential on the vibrational spectra.

For the purposes of measuring the positions and integrating the intensities of the two VDOS peaks of interest despite the $\sim$27 cm^{-1} resolution, we interpolated between data points for the appropriate portions of each spectra. The positions of the δDOD peaks were sensitive to both φ and the layer. These data are shown in Fig. S19. In layer 1, the peak occurs at a higher frequency at all non-zero φ, as discussed in the main text. We observed blue shifts of this vibrational mode's frequency in layer 1 was up to about 10 cm^{-1} at modest positive and negative φ. Layer 2 demonstrated very little effect of φ on the δDOD peak position and the δDOD peak position in layer 3 appeared to blue shift with increasing φ. Moreover, the position of the δDOD peak in layer 1 was red-shifted relative to those of layers 2 an 3. This is characteristic of water with a weakened hydrogen bonding network,[6] consistent with the observation of the least number of hydrogen bonds formed on average in layer 1 (Figs. S5-S7).

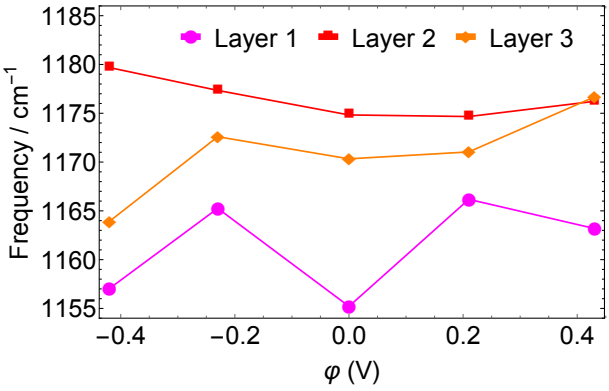

Figure S19: Positions of the water δDOD peaks for each φ and layers 1-3 as determined by the maximum values of the interpolating functions in this region of the spectra.

The positions of the water νOD peaks for each φ and layers 1-3 were also determined via interpolation are shown in Fig. S20. We only investigated the global maxima of the interpolating functions for each spectrum despite there likely being several characteristic νOD peaks.[7–9] These data also demonstrate that in layer 1 the position of the peak was blue-shifted at all non-zero φ, with shifts of the positions of maximum frequency of over 100 cm^{-1}. There was no discernible pattern in the νOD peak positions beyond layer 1.

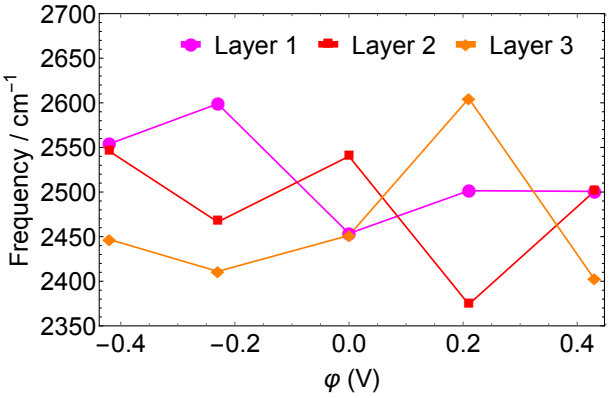

Figure S20: Positions of the water νOD peaks for each φ and layers 1-3 as determined by the maximum values of the interpolating functions in this region of the spectra.

We also integrated the total intensities of the δDOD peaks using the interpolated spectra. These integrated intensities are shown in Fig. S21. For layer 1, we observed a minimum integrated spectral intensity for δDOD at the PZC, which was also observed for SEIRAS spectra of aqueous electrolytes on Au(111).[7] We observed a maximal integrated

δDOD peak intensity at the most negative φ studied. There were no discernible patterns observed among the integrated intensities of the δDOD peaks in layers 2 and 3.

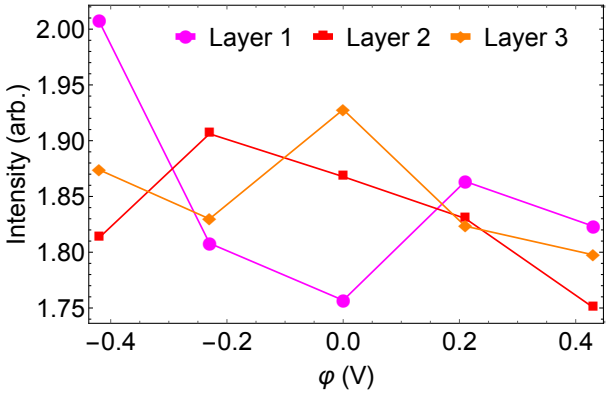

Figure S21: Integrated intensities (arbitrary units) of the water δDOD peaks for each φ and layers 1-3. The integration range was 1000-1400 cm^{-1}.

For comparison, we also computed the VDOS spectra from the velocity autocorrelation functions only in the surface-normal dimension z given the importance of surface-normal dipoles in many surface-enhanced spectroscopies. These are shown alongside their corresponding 3D VDOS spectra in Figs. S22-S24. For the most part, the z-only VDOS spectra hew closely to the full VDOS spectra, especially in the second and third layers. In layer 1, the z-only VDOS spectra demonstrate some subtle differences from the 3D spectra: The δDOD peaks appear slightly red-shifted in the z-only spectra relative to the full spectra. In addition, the z-only spectra for layer 1 generally hew to only the second νOD peaks of the full spectra for $\varphi \neq 0$ V. That this is more evident when there is a non-zero potential is consistent with the observation of water molecules that are more oriented along the surface-normal electric fields associated with the applied biases. This difference between the full and z-only spectra furthermore suggests that there are more than one characteristic νOD mode in this heterogeneous environment. However, it is likely that all vibrational modes are strongly coupled between the (arbitrary) Cartesian dimensions given the overall similarities between the spectra.

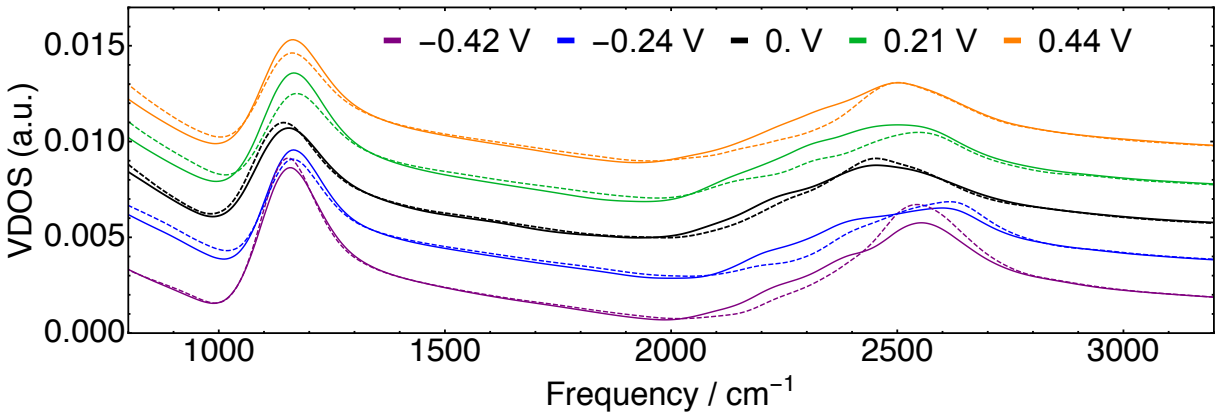

Figure S22: Layer 1 water VDOS spectra obtained from the 3D velocity autocorrelation functions (solid; same as main text) and from the z velocity autocorrelation functions (dashed). The spectra for each φ are shifted arbitrarily for clarity.

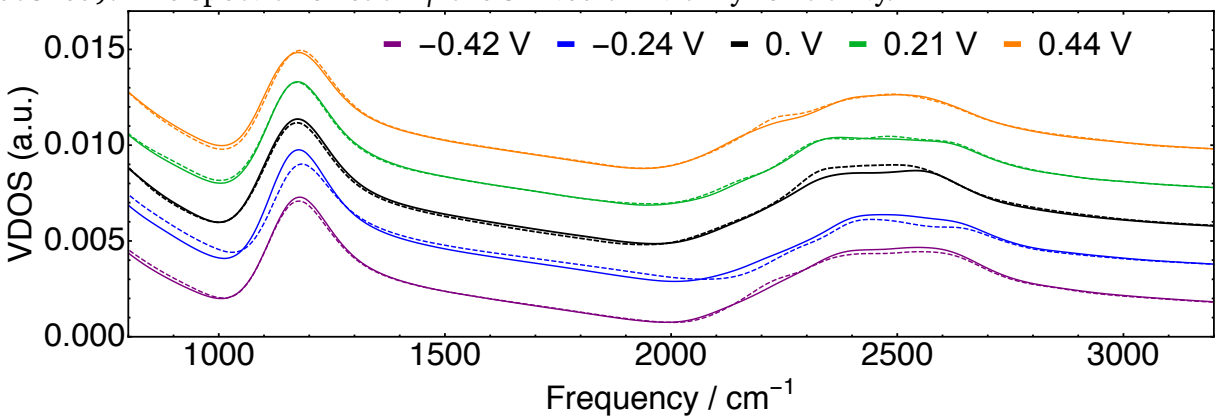

Figure S23: Layer 2 water VDOS spectra obtained from the 3D velocity autocorrelation functions (solid; same as main text) and from the z velocity autocorrelation functions (dashed). The spectra for each φ are shifted arbitrarily for clarity.

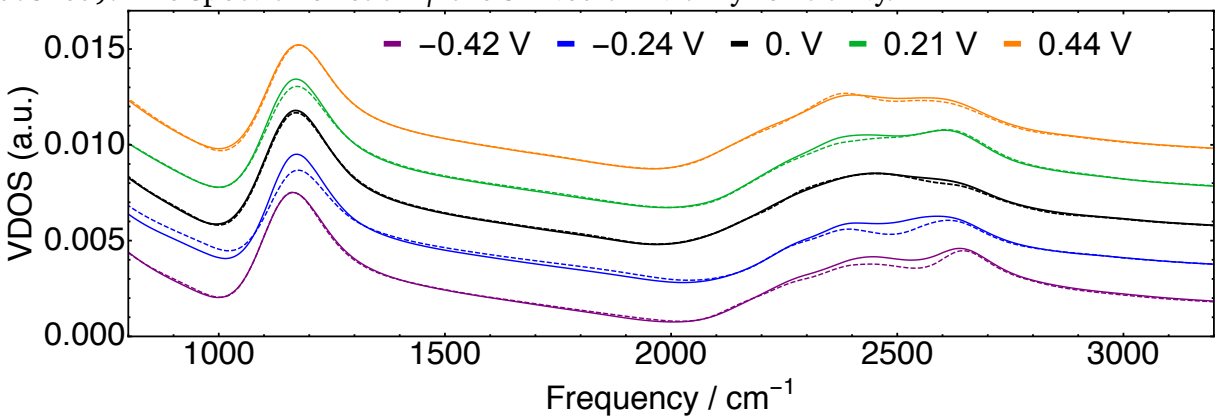

Figure S24: Layer 3 water VDOS spectra obtained from the 3D velocity autocorrelation functions (solid; same as main text) and from the z velocity autocorrelation functions (dashed). The spectra for each φ are shifted arbitrarily for clarity.

The integrated intensities of the δDOD peaks for the 3D and z-only VDOS spectra for layer 1 water are shown in Fig. S25. These integrals show discrepancies only at positive φ, and for the z-only spectra the integrated intensity is no longer minimal at PZC.

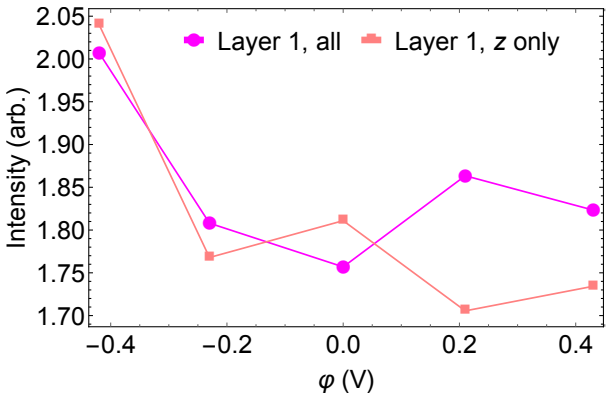

Figure S25: Integrated intensities (arbitrary units) of the water δDOD peaks in the 3D (magenta) and z-only (light pink) VDOS spectra for layer 1 water.

6 Representative input files and initial Cartesian coordinates

Example `Quantum-ESPRESSO`[10,11] `PWscf` input file, including initial coordinates, for the σ = -0.4 e trajectory:

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   calculation  = 'md',
   max_seconds = 3520,
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   pseudo_dir = '/home/zkg/ONCV-pseudos/',
   etot_conv_thr = 1.0D-4,
   forc_conv_thr = 1.0D-3,
   dt = 10.0,
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   tefield = .true.,
   dipfield = .true.,
   gate = .true.,
/
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!   celldm(1) = 7.89223,
   nspin       = 1,
   tot_charge  = -0.4,
```

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   ntyp        = 3,
   ecutwfc     = 60,
   occupations = 'smearing', smearing = 'cold', degauss = 0.01,
   edir = 3,
   emaxpos = 0.99,
   eopreg = 0.95,
   zgate = 0.87,
   block = .true.,
   block_1 = 0.743665,
   block_2 = 0.91,
   block_height = 0.25,
/
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   mixing_mode = 'plain',
   mixing_beta = 0.5D0,
   startingwfc = 'file',
   startingpot = 'file',
   electron_maxstep = 150,
/
&IONS
   ion_dynamics = 'verlet',
   pot_extrapolation = 'first_order',
   wfc_extrapolation = 'none',
   ion_temperature = 'rescaling',
   tempw = 330.D0,
   tolp = 100.D0,
/
 K_POINTS { gamma }

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 H  2.00 H_ONCV_PBE-1.0.UPF
 O  15.999 O_ONCV_PBE-1.0.UPF

 CELL_PARAMETERS (angstrom)
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   0.000000000    11.808773755    0.000000000
   0.000000000    0.000000000    36.000000000

ATOMIC_POSITIONS (angstrom)
Au       5.113345000   0.000000000   6.410460000    1   1   0
Au       7.670027730   1.476096250   6.410460000    1   1   0
Au       5.113345000   2.952192500   6.410460000    1   1   0
Au       7.670027730   4.428288750   6.410460000    1   1   0
Au       5.113345000   5.904385000   6.410460000    1   1   0
Au       7.670027730   7.380481250   6.410460000    1   1   0
Au       5.113345000   8.856577500   6.410460000    1   1   0
Au       7.670027730  10.332673750   6.410460000    1   1   0
Au       0.000000000   0.000000000   6.410460000    1   1   0
Au       2.556672500   1.476096250   6.410460000    1   1   0
Au       0.000000000   2.952192500   6.410460000    1   1   0
Au       2.556672500   4.428288750   6.410460000    1   1   0
```

Au	0.000000000	5.904385000	6.410460000	1	1	0
Au	2.556672500	7.380481250	6.410460000	1	1	0
Au	0.000000000	8.856577500	6.410460000	1	1	0
Au	2.556672500	10.332673750	6.410460000	1	1	0
Au	6.817796740	0.000000000	8.820910000			
Au	9.374469240	1.476096250	8.820910000			
Au	6.817796740	2.952192500	8.820910000			
Au	9.374469240	4.428288750	8.820910000			
Au	6.817796740	5.904385000	8.820910000			
Au	9.374469240	7.380481250	8.820910000			
Au	6.817796740	8.856577500	8.820910000			
Au	9.374469240	10.332673750	8.820910000			
Au	1.704451740	0.000000000	8.820910000			
Au	4.261124240	1.476096250	8.820910000			
Au	1.704451740	2.952192500	8.820910000			
Au	4.261124240	4.428288750	8.820910000			
Au	1.704451740	5.904385000	8.820910000			
Au	4.261124240	7.380481250	8.820910000			
Au	1.704451740	8.856577500	8.820910000			
Au	4.261124240	10.332673750	8.820910000			
Au	8.522248480	0.000000000	11.231400000			
Au	5.965575980	1.476096250	11.231400000			
Au	8.522248480	2.952192500	11.231400000			
Au	5.965575980	4.428288750	11.231400000			
Au	8.522248480	5.904385000	11.231400000			
Au	5.965575980	7.380481250	11.231400000			
Au	8.522248480	8.856577500	11.231400000			
Au	5.965575980	10.332673750	11.231400000			
Au	3.408903480	0.000000000	11.231400000			
Au	0.852224850	1.476096250	11.231400000			
Au	3.408903480	2.952192500	11.231400000			
Au	0.852224850	4.428288750	11.231400000			
Au	3.408903480	5.904385000	11.231400000			
Au	0.852224850	7.380481250	11.231400000			
Au	3.408903480	8.856577500	11.231400000			
Au	0.852224850	10.332673750	11.231400000			
O	3.474117948	8.795442378	23.759914278			
H	3.580137747	7.833496774	23.644781550			
H	2.541373385	8.908932147	23.993603612			
O	4.097545029	4.670815939	20.864088030			
H	3.303533920	4.115978906	20.873095898			
H	4.764900793	4.050070607	20.505774890			
O	2.909112584	8.542762202	17.217268989			
H	3.396052387	7.683220980	17.289893722			
H	2.312305576	8.508994790	16.416936571			
O	0.232576032	4.304460875	21.044962170			
H	0.685409235	3.895099936	21.810698945			
H	0.571792465	3.830027377	20.266290198			
O	2.040303802	9.224822479	21.022950338			
H	2.565430742	8.461253552	20.633679016			
H	2.440159050	9.357660497	21.894829355			
O	3.814232983	7.519272386	14.513869883			
H	3.861329045	6.691738014	15.054334810			
H	3.740420357	7.178721275	13.597302711			

O	6.372340906	0.265112696	23.893133426
H	5.401910234	0.217797787	23.682628134
H	6.679893432	11.179966408	24.094196551
O	4.220965709	-0.176050516	20.319718578
H	4.692675309	10.894684643	20.764021238
H	4.202641997	11.262390154	19.398979807
O	7.544226760	0.889303664	21.167276374
H	7.550907232	11.950356118	20.530269816
H	7.160889424	0.521074027	21.987596008
O	9.520324557	10.907996425	17.499028659
H	9.119505344	10.022315900	17.478372402
H	10.378123927	10.706331695	17.967552255
O	7.057798133	3.496010800	14.239344392
H	7.522008043	2.657973188	14.445831953
H	6.131383448	3.208599843	14.119938950
O	1.316554946	6.078698394	17.807896839
H	1.411752746	5.094069298	17.867492623
H	1.799365568	6.313255009	16.994560159
O	6.964224186	5.638285124	18.402485431
H	7.063309904	5.228603389	19.288894212
H	7.650686725	5.141886460	17.897061519
O	1.374760486	0.186536196	21.752680832
H	1.979165213	11.367126349	21.312694192
H	0.546023664	11.458713054	21.949312025
O	5.718377755	2.451498745	20.054612051
H	6.536171900	1.994654616	20.410696562
H	5.224502671	1.674258688	19.740957774
O	0.139373805	11.588654048	15.030676216
H	9.955235187	10.890480477	14.475285318
H	10.144621478	11.323276223	15.958870780
O	5.595215230	5.079985481	24.009202964
H	6.192947186	4.297157976	23.878971613
H	4.730787563	4.771495114	23.692189825
O	9.271246580	5.057606768	15.084525031
H	9.139373221	4.547263376	15.940084413
H	9.107189335	4.340538749	14.442245290
O	7.581470036	4.565547285	20.906279431
H	8.507896889	4.262196823	20.993705173
H	7.026950669	3.856038514	21.283633403
O	9.342530662	10.659257278	22.282439888
H	8.884247195	10.664727801	21.415891407
H	9.204037211	9.708367678	22.549106189
O	9.774618942	2.470147379	14.470125608
H	9.761951375	2.119886756	13.553747240
H	9.606122098	1.674678834	15.014409472
O	8.283864260	1.442263302	18.298522480
H	8.778400838	0.644924907	18.006819780
H	7.361433622	1.201987614	18.009057856
O	8.594941225	9.902049310	13.808871968
H	7.617121688	9.936032829	13.788288235
H	8.746493239	9.036083611	14.285667702
O	1.636095822	10.491308013	18.601769700
H	2.071304724	9.713494133	18.160454727
H	1.717330182	10.277477030	19.558269276

O	8.784266081	8.106721185	22.922853506
H	7.861763259	7.871519202	22.656446073
H	9.297933137	7.791784221	22.132015071
O	6.817099986	8.348986720	18.081828776
H	6.776928047	7.387478443	18.326417907
H	7.702839380	8.352776968	17.656090659
O	1.104121552	8.635969590	15.292988970
H	1.248163681	7.739032244	14.848938860
H	0.184883987	8.592578060	15.616902938
O	10.082773089	7.106578078	20.737625620
H	0.763857614	7.480847628	20.760174626
H	0.006667415	6.136304498	20.700411653
O	5.340199259	11.240343292	14.919425159
H	5.731463722	10.363702969	14.680736780
H	4.368268790	11.058479676	14.892990557
O	7.187144861	2.890747058	23.681981996
H	8.090164596	2.938748766	24.021221265
H	6.928916285	1.939348005	23.735326136
O	4.777842333	10.245507241	18.053635333
H	5.535400463	9.616309354	18.075549348
H	4.068274911	9.715128541	17.606037243
O	4.643734084	3.352721579	17.488688572
H	4.650260212	2.532359508	16.956464823
H	5.321849959	3.189297114	18.169821351
O	1.357360322	6.196853128	14.571333565
H	0.527620207	5.693428033	14.813738514
H	1.686111298	5.775095878	13.750884539
O	8.701776102	7.718298499	15.292727958
H	7.742451933	7.537135286	15.367479610
H	9.037741243	6.817169423	15.072826087
O	9.969677435	5.427750273	24.025243758
H	10.273246478	4.508601130	23.928956051
H	9.825442120	5.739686861	23.120100759
O	2.188042221	1.037771562	17.156754963
H	2.406764988	0.773520384	16.245266186
H	2.044255473	12.029971974	17.683522319
O	6.108185019	8.772426972	14.332849826
H	6.512709617	7.998699955	13.882821341
H	5.206968795	8.377721544	14.512851591
O	2.407504330	2.337531190	20.368124086
H	1.820377219	1.626642689	20.719900776
H	3.211567483	1.860979536	20.111648467
O	4.710720305	2.125566874	14.820277806
H	5.119816000	1.254770380	14.663086060
H	3.763570969	1.928102807	14.656994079
O	5.928667169	0.732223829	17.371483246
H	6.091221470	12.376808279	16.426037003
H	5.453171943	11.708238437	17.622063179
O	3.915635019	0.708999047	23.001575333
H	2.982259975	0.458710579	23.117727809
H	4.057554913	0.651962033	22.034145573
O	4.187830893	4.865685626	14.830041757
H	4.624640332	4.175668730	15.364559229
H	3.350304101	4.430239194	14.530929367

```
O         2.734930166   6.912155050  20.123100889
H         2.342701406   6.707709944  19.241110277
H         3.426032423   6.216702418  20.243083337
O         5.215148398   9.245526769  21.556350353
H         4.671907214   9.283395995  22.369309437
H         5.530929727   8.306644976  21.524715444
O         1.034654221   2.574185280  23.336568339
H         1.203145716   1.776481719  22.785872268
H         0.399288146   2.259355231  23.996447712
O         2.960577986  10.250997397  14.322452975
H         2.097855703   9.960546212  14.703456519
H         3.338466165   9.402438925  14.032273083
O         2.318035393   0.982402524  14.210167537
H         2.700310798   0.187608399  13.784531538
H         1.416799019   0.652175916  14.483836850
O         9.519799416   8.071971769  18.075852980
H         9.574320183   7.863576501  19.032485268
H        10.030791243   7.336541678  17.684751977
O         6.437874476   6.879296944  22.015009570
H         6.913604910   6.204263999  21.477493482
H         6.090332561   6.331210333  22.761748149
O         7.536596241  10.031564962  20.211838393
H         6.765485488   9.800110846  20.770287063
H         7.405208096   9.484800858  19.399728936
O         6.593252890   6.157429864  14.402972366
H         5.662517227   5.851047496  14.418310548
H         7.083337222   5.306785394  14.368605413
O         1.962559959   3.590632904  14.008047808
H         2.185224005   2.739006292  13.579945928
H         1.097275312   3.358570465  14.431524385
O         4.320369268   6.147603890  17.444023372
H         5.272127100   6.125501049  17.670962284
H         4.142719942   5.189664553  17.317894939
O         1.335442762   3.382910157  18.114275868
H         1.837484628   3.083071404  18.909505056
H         1.548836692   2.613279755  17.520719692
O         7.594248263   0.772338415  14.536015698
H         8.263070039  11.932337678  14.267258595
H         6.742224287   0.298724870  14.444621387
O         8.945901579   3.860722780  17.442625259
H         8.586300400   2.941156546  17.655562648
H         9.871368663   3.798414073  17.783055100
```

Accompanying `Environ`[12,13] input file for the σ = -0.4 e trajectory:

```
 &ENVIRON
   !
   verbose = 2
   environ_thr = 1.d-1
   environ_type = 'input'
   env_electrostatic = .true.
   env_static_permittivity = 78.3D0
   env_dielectric_regions = 1
```

```
   !
 /
 &BOUNDARY
   solvent_mode = 'electronic'
   solvent_radius = 7.0D0,
 /
 &ELECTROSTATIC
   !
   pbc_correction = 'none'
   pbc_dim = 2
   pbc_axis = 3
   !
   tol = 1.d-7
   mix = 0.6
   solver = 'iterative'
   auxiliary = 'full'
   !
 /
DIELECTRIC_REGIONS {angstrom}
1.0   1.0   5.5   5.5  6.4104    6.4104   0.5   2   3
```

Initial coordinates of the σ = -0.2 e trajectory:

```
Au       5.113345000   0.000000000   6.410460000
Au       7.670027730   1.476096250   6.410460000
Au       5.113345000   2.952192500   6.410460000
Au       7.670027730   4.428288750   6.410460000
Au       5.113345000   5.904385000   6.410460000
Au       7.670027730   7.380481250   6.410460000
Au       5.113345000   8.856577500   6.410460000
Au       7.670027730  10.332673750   6.410460000
Au       0.000000000   0.000000000   6.410460000
Au       2.556672500   1.476096250   6.410460000
Au       0.000000000   2.952192500   6.410460000
Au       2.556672500   4.428288750   6.410460000
Au       0.000000000   5.904385000   6.410460000
Au       2.556672500   7.380481250   6.410460000
Au       0.000000000   8.856577500   6.410460000
Au       2.556672500  10.332673750   6.410460000
Au       6.817796740   0.000000000   8.820910000
Au       9.374469240   1.476096250   8.820910000
Au       6.817796740   2.952192500   8.820910000
Au       9.374469240   4.428288750   8.820910000
Au       6.817796740   5.904385000   8.820910000
Au       9.374469240   7.380481250   8.820910000
Au       6.817796740   8.856577500   8.820910000
Au       9.374469240  10.332673750   8.820910000
Au       1.704451740   0.000000000   8.820910000
Au       4.261124240   1.476096250   8.820910000
Au       1.704451740   2.952192500   8.820910000
Au       4.261124240   4.428288750   8.820910000
Au       1.704451740   5.904385000   8.820910000
Au       4.261124240   7.380481250   8.820910000
```

Au	1.704451740	8.856577500	8.820910000
Au	4.261124240	10.332673750	8.820910000
Au	8.522248480	0.000000000	11.231400000
Au	5.965575980	1.476096250	11.231400000
Au	8.522248480	2.952192500	11.231400000
Au	5.965575980	4.428288750	11.231400000
Au	8.522248480	5.904385000	11.231400000
Au	5.965575980	7.380481250	11.231400000
Au	8.522248480	8.856577500	11.231400000
Au	5.965575980	10.332673750	11.231400000
Au	3.408903480	0.000000000	11.231400000
Au	0.852224850	1.476096250	11.231400000
Au	3.408903480	2.952192500	11.231400000
Au	0.852224850	4.428288750	11.231400000
Au	3.408903480	5.904385000	11.231400000
Au	0.852224850	7.380481250	11.231400000
Au	3.408903480	8.856577500	11.231400000
Au	0.852224850	10.332673750	11.231400000
O	3.392863129	8.809062166	23.694277586
H	3.430799695	7.839672957	23.699482202
H	2.626849334	9.025043682	24.247672842
O	4.100611148	4.608363981	20.958175486
H	3.305030210	4.076227276	21.104107817
H	4.720366595	3.941982484	20.572508445
O	2.935248419	8.581025711	17.307817174
H	3.415418403	7.718988414	17.427422307
H	2.313723223	8.502514644	16.541552606
O	0.043767103	4.235117830	21.080796629
H	0.326780003	3.663175735	21.839836725
H	0.446468981	3.846553181	20.283516859
O	2.053216842	9.154859539	21.151462693
H	2.554193247	8.429780061	20.687025652
H	2.403155132	9.145631908	22.070556559
O	3.853716830	7.542815393	14.472981998
H	3.907300409	6.706933215	14.999745493
H	3.781369607	7.217562682	13.550791354
O	6.473315818	0.334455691	23.730797688
H	5.489615292	0.354077254	23.613836238
H	6.688796059	11.284056986	24.128080726
O	4.286365818	-0.170391849	20.270686922
H	4.682366286	10.933117828	20.826425418
H	4.312497523	11.178936379	19.385526174
O	7.524145072	1.010448944	21.159860074
H	7.519535202	12.049645367	20.550862367
H	7.217591943	0.648071430	22.019052206
O	9.650007722	10.857217229	17.519543852
H	9.279748643	9.956753942	17.555849014
H	10.462272859	10.747492044	18.093434563
O	6.963775444	3.437084455	14.019763645
H	7.476723509	2.639431914	14.265397769
H	6.035444876	3.137927626	14.172662914
O	1.329990906	6.008963153	17.708314185
H	1.439540820	5.023047747	17.834389378
H	1.725984397	6.195214516	16.835494068

O	6.926793040	5.628968384	18.481327681
H	7.007642900	5.213697184	19.370352132
H	7.613598452	5.135907020	17.970201902
O	1.316216476	0.185395956	21.802899021
H	1.952418702	11.356222185	21.435172873
H	0.474874147	11.441362857	21.948713118
O	5.622012454	2.436962203	19.976765160
H	6.450571807	2.070638301	20.402117659
H	5.126813352	1.600497822	19.851215938
O	-0.008905920	11.608006841	15.053907039
H	9.833822714	10.885075591	14.496058497
H	10.077150175	11.283038586	15.990474517
O	5.528242653	5.116966923	24.070739598
H	6.121384421	4.326029090	23.965354383
H	4.686313923	4.853352377	23.663944226
O	9.255197468	5.103843294	15.195698020
H	9.079881481	4.656453434	16.082406413
H	9.078323586	4.354410241	14.594598157
O	7.596080062	4.635257600	21.011763902
H	8.565895657	4.447180378	20.940339315
H	7.234783876	3.844400687	21.447387692
O	9.357856864	10.691429072	22.278343105
H	8.817783639	10.593623132	21.460746789
H	9.297614336	9.779554327	22.659371911
O	9.824590544	2.516453493	14.447823756
H	9.810996843	2.201957951	13.515122005
H	9.672774004	1.687898062	14.947470257
O	8.268927126	1.491772945	18.164085701
H	8.819579384	0.713024541	17.946563594
H	7.339351085	1.196165445	17.963693050
O	8.724775263	9.698252297	13.752235477
H	7.762307946	9.814977406	13.631640597
H	8.767108227	8.843797781	14.280031167
O	1.764631539	10.526622372	18.679232030
H	2.087374875	9.706718072	18.216716035
H	1.806512004	10.293991924	19.632245159
O	8.853747948	8.069654454	22.951234712
H	7.927049371	7.751061533	22.800270443
H	9.309255230	7.733396344	22.132968847
O	6.989953918	8.365873024	18.116662787
H	6.770824868	7.441304356	18.378438980
H	7.955520514	8.241522690	17.894974801
O	1.053967993	8.645789514	15.382081884
H	1.209663668	7.800699039	14.860895591
H	0.132225488	8.526715978	15.681775221
O	10.139208894	7.116857470	20.782128882
H	0.784326853	7.563713795	20.860579526
H	0.105728238	6.155229322	20.794425456
O	5.277516347	11.160116836	14.952820512
H	5.768883669	10.326974559	14.761892774
H	4.326823362	10.891478025	14.841257633
O	7.151405578	2.944582173	23.794734224
H	8.063446340	3.011237069	24.117787306
H	6.896383048	1.991081299	23.877506162

O	4.833740704	10.182384347	18.075760863
H	5.574640884	9.535435308	18.091168790
H	4.101036981	9.699402220	17.609561812
O	4.640576997	3.430735589	17.449023897
H	4.689656317	2.580093169	16.968742864
H	5.234367614	3.293534498	18.216416266
O	1.301738483	6.244361599	14.519611271
H	0.495178586	5.699301083	14.746449206
H	1.642919204	5.924235685	13.663121791
O	8.660042215	7.646253398	15.385727268
H	7.698730112	7.693409396	15.538787617
H	8.804730382	6.684030095	15.161060350
O	9.992294434	5.418866357	24.216578156
H	10.385356181	4.571448828	23.965888171
H	9.731877907	5.849802218	23.376351002
O	2.184738151	1.076672189	17.143034130
H	2.484589706	0.873941766	16.236373635
H	2.134615796	12.045708620	17.645994564
O	6.164821123	8.744008270	14.273897966
H	6.603899431	7.903979023	14.007306064
H	5.256284665	8.364930273	14.462768238
O	2.374970330	2.272384315	20.377070106
H	1.779779073	1.579282052	20.760715776
H	3.122892480	1.760744124	20.025151046
O	4.706552609	2.082140192	14.737238647
H	5.009390909	1.152971108	14.742271035
H	3.743982159	1.989939913	14.595946964
O	5.822322324	0.766471908	17.348765278
H	6.097454687	12.415667891	16.429297543
H	5.439051150	11.689585249	17.584935128
O	3.945207262	0.769331980	23.055927912
H	3.072211441	0.406648161	23.280526747
H	3.997057137	0.724882984	22.083005228
O	4.178642057	4.896436028	14.943871056
H	4.529915034	4.338363411	15.668112044
H	3.428019178	4.373828635	14.565870709
O	2.711528955	6.851562392	20.038307922
H	2.350208519	6.661800239	19.141663349
H	3.384199253	6.142353793	20.172114482
O	5.298105298	9.300251875	21.714208869
H	4.683895268	9.340819350	22.472340910
H	5.601847424	8.358082246	21.694625926
O	1.061773826	2.622755182	23.264207119
H	1.223514792	1.803345786	22.746677949
H	0.490434708	2.312810572	23.984661182
O	2.908032562	10.198402535	14.356352042
H	2.095751486	9.861582142	14.814763702
H	3.294953875	9.378479541	14.001965588
O	2.254508302	0.926409089	14.251154321
H	2.656621750	0.136629576	13.835662191
H	1.368259697	0.563006212	14.530162786
O	9.601585439	8.042264530	18.169993824
H	9.675626063	7.845251846	19.132496679
H	10.064099513	7.276759403	17.770901390

O	6.511785937	6.858680157	22.168856232
H	6.915481590	6.171232744	21.580777368
H	6.080576255	6.296940853	22.866949849
O	7.491547808	10.140862092	20.254360561
H	6.778815182	9.909798768	20.890372087
H	7.368491283	9.499100256	19.510204876
O	6.562176495	6.125539028	14.299793150
H	5.645246329	5.784401882	14.390471858
H	7.082562613	5.294134937	14.285570749
O	1.990671462	3.599797976	13.948932693
H	2.191071726	2.709355297	13.583077951
H	1.146612387	3.398942355	14.428755345
O	4.369673646	6.247919763	17.483694310
H	5.297479272	6.108315818	17.778203041
H	4.060848038	5.329108943	17.358884859
O	1.328804172	3.414979642	18.159122664
H	1.795740487	3.063743493	18.960224625
H	1.538678698	2.672561728	17.536195169
O	7.567350980	0.752360432	14.542420580
H	8.297254609	11.923804937	14.614202639
H	6.768183665	0.222694492	14.341589562
O	8.880130541	3.919271359	17.517617612
H	8.567605006	2.955303556	17.626661670
H	9.798259779	3.880242941	17.866917282

Initial coordinates of the $\sigma = 0$ e trajectory:

Au	5.173900970	0.285728353	6.410460002
Au	7.867060373	1.441943922	6.410460002
Au	5.365586323	3.177701420	6.410460002
Au	7.666171977	4.526538966	6.410460002
Au	5.044124624	6.001230585	6.410460002
Au	7.558271223	7.427015365	6.410460002
Au	5.159361938	9.121919196	6.410460002
Au	7.565397734	10.442693153	6.410460002
Au	−0.072087954	0.021347949	6.410460002
Au	2.429646017	1.326647058	6.410460002
Au	0.036836371	3.202833250	6.410460002
Au	2.701797208	4.395996953	6.410460002
Au	−0.107874575	6.001697787	6.410460002
Au	2.599128080	7.433233039	6.410460002
Au	−0.168108525	8.959495892	6.410460002
Au	2.403573037	10.269330105	6.410460002
Au	7.015335516	0.015058390	8.921855987
Au	9.690183836	1.453864232	9.114868978
Au	7.249581800	2.896182233	8.808896377
Au	9.634691706	4.489380036	8.947297284
Au	7.038029855	5.734501999	9.492410842
Au	9.412766271	7.486525446	8.782613508
Au	6.912689379	8.518094413	8.914351224
Au	9.504088221	10.237350958	9.314531462
Au	1.800434634	0.069655412	9.246583933
Au	4.144759654	1.603168820	8.675883287

Au	1.764530467	3.078055149	8.993907110
Au	4.086503282	4.839254567	9.055110462
Au	1.686070621	6.072160831	9.325722468
Au	4.377161651	7.532368313	8.977160752
Au	1.839265031	8.838554578	8.956663629
Au	4.472211833	10.508957365	8.826595489
Au	8.635128323	0.205027685	11.576325584
Au	5.954833128	1.569672365	11.177984181
Au	8.763703432	3.036807829	11.490679173
Au	6.289314339	4.527271719	11.778614617
Au	9.076778832	5.847181437	11.386464080
Au	6.104409591	7.503080634	11.883268699
Au	8.855262244	8.666131095	11.625134856
Au	6.475582647	10.229102488	10.949244218
Au	3.617353122	0.047182182	11.427538071
Au	0.976814991	1.427149227	11.768732591
Au	3.444206134	2.985428643	11.452206375
Au	1.053711680	4.236637329	12.177320074
Au	3.520274178	5.908511220	11.876204857
Au	1.043527467	7.552150415	12.144223869
Au	3.479839596	8.797599951	11.349725118
Au	1.180310727	10.492417734	11.870165344
O	4.628732129	10.637647071	25.357315063
H	4.980119175	11.459900542	25.724934850
H	4.678601920	9.893220529	26.015379049
O	4.147480683	2.668430261	21.831215545
H	3.312081191	2.735742495	21.280910260
H	4.763791502	2.266558237	21.123564108
O	2.578961909	8.374572224	18.460450255
H	2.324726601	7.445172775	18.757003670
H	1.969973272	8.257548450	17.637798057
O	0.343876493	4.247644152	22.151661449
H	0.841188174	4.080750390	23.020870920
H	0.702445209	3.583851246	21.530750848
O	4.436427674	10.667412428	22.493821635
H	4.039357435	9.775704487	22.478128748
H	4.662921483	10.692845005	23.434352478
O	4.640049987	5.848778520	15.863059123
H	4.756820773	5.676425979	16.814303610
H	4.153640518	5.088369680	15.528365512
O	8.956248841	0.974569372	26.345007116
H	8.394799911	0.464911815	25.711440531
H	9.245871664	13.593233199	25.930725885
O	5.952300734	-0.808652523	20.199403058
H	5.575367497	10.737430531	21.042623188
H	5.613015768	10.306771833	19.572654703
O	7.967002725	1.860099564	20.811101180
H	8.582051899	13.248782333	20.136627922
H	7.962714341	1.215159018	21.588165159
O	8.933069366	9.170565698	20.684789458
H	8.604071329	8.451920885	19.998762318
H	9.913848335	9.369358752	20.450776494
O	6.122239004	1.217670579	14.443742860
H	6.886097961	0.654697586	14.334926965

H	5.336033234	0.709336503	14.095992105
O	0.930527190	4.486536465	17.586099790
H	0.144632243	3.935756735	17.493859620
H	1.249701582	4.592671841	16.669398648
O	7.248755798	4.833896080	18.541366465
H	7.603810340	4.694177329	19.465138264
H	7.655471228	4.042749394	18.124447202
O	2.162237841	-0.124970478	21.234109422
H	3.079516317	11.674197624	21.566845018
H	1.522265531	11.833132814	22.011082054
O	5.626374724	1.824307990	19.866219732
H	6.603834288	1.988291140	20.175910812
H	5.571344920	0.825282443	19.942950454
O	0.576069496	11.302009790	17.446648245
H	9.814600797	11.269285691	17.362855364
H	10.788021414	10.725035520	18.303323587
O	6.265158232	6.234045200	22.744571647
H	5.733415717	5.772747134	23.434367591
H	5.708816897	6.312874768	21.941660530
O	8.867423324	4.854729148	14.381319618
H	8.791134829	3.911042169	14.351024350
H	9.247951274	4.956512494	13.495113684
O	8.207059133	5.302567252	20.970701492
H	9.064914871	5.128297697	21.379687459
H	7.633044258	5.573090314	21.732279439
O	10.880352415	12.196565134	23.115128212
H	9.978481759	11.925311370	22.735529358
H	10.937735727	11.452735607	23.714853933
O	8.928654199	2.147204557	14.854833326
H	8.594436062	1.419760898	14.330755146
H	8.631613435	2.222338480	15.805110456
O	8.177048907	-0.871629142	17.696046648
H	8.003558383	-1.134096999	18.635810028
H	7.642658501	-1.514342013	17.224436578
O	9.617876436	9.153628434	15.025097060
H	9.912789032	8.649973173	14.260992399
H	8.694271201	8.682213299	15.212660694
O	1.059487048	9.716508213	19.947634735
H	1.578420125	9.226805432	19.234852193
H	1.638793192	10.363878874	20.465734805
O	10.356059809	8.431276024	25.278778062
H	9.681474000	7.903293959	24.752943046
H	10.871160898	8.791970295	24.548647670
O	8.605127329	7.375965169	18.390586512
H	8.195581540	6.488458101	18.488754845
H	9.505812399	7.170585243	18.113937479
O	0.903902547	7.654699701	16.780457922
H	1.245702437	6.904773061	16.186473285
H	0.430838317	8.318904861	16.141898043
O	12.181140212	6.916444423	22.835605726
H	2.609181937	6.391237108	22.308341142
H	1.199417800	6.294103191	22.825220571
O	5.962666929	9.789913444	14.086203817
H	5.258909737	9.389116261	14.634592212

H	5.493132499	9.945763053	13.262319632
O	4.864851867	5.144803737	24.880664334
H	5.435417844	4.837294811	25.598001983
H	4.194400784	4.407261585	24.791655138
O	5.072086630	9.166811181	18.411987682
H	5.817070760	8.595372627	18.092453848
H	4.190448684	8.790630887	18.573296931
O	5.461209717	2.023262220	17.324967854
H	5.528461825	1.110872600	16.970996723
H	5.463641165	1.934618782	18.383219570
O	1.389603339	5.560985638	15.008775586
H	0.392049072	5.551427043	14.883100162
H	1.803135686	5.601460425	14.130620945
O	7.301776451	8.563016974	16.257386411
H	7.686522833	7.984749326	16.947098014
H	7.008400569	7.995672379	15.499962510
O	11.460702595	5.661797697	26.320099082
H	11.345876656	6.581163227	26.006417497
H	10.562955294	5.321059973	26.192794454
O	2.614795005	1.686439085	17.697699805
H	3.310847786	2.345948368	17.519608356
H	3.056166781	12.581683271	17.601939955
O	6.679745442	6.775569503	14.444350221
H	7.415189752	6.140063594	14.300243852
H	6.046153465	6.092540788	14.758132373
O	1.736611530	2.520357943	20.085141247
H	1.903672973	1.610527533	20.507954906
H	2.035736041	2.173390887	19.193021764
O	3.469805714	0.162756513	13.929125357
H	2.823174678	0.767420830	14.371506197
H	3.193756403	-0.650308706	14.416581682
O	3.916174766	-0.519524961	17.139993149
H	3.377145022	10.801241011	16.472381056
H	4.351816014	10.613196324	17.730288859
O	6.821730972	2.056068876	24.101912535
H	6.278266364	2.328967505	23.371895617
H	7.366979164	2.807547008	24.356207345
O	3.735595426	3.375517193	15.577399690
H	4.393880221	2.939024777	16.135178081
H	3.119803539	2.701953063	15.212485020
O	4.298233665	5.725131522	21.183154901
H	4.456383564	5.521105922	20.234795349
H	4.240886884	4.806786690	21.471993452
O	7.386803923	10.622207952	24.635492882
H	6.413919859	10.597146388	24.688067085
H	7.637654980	9.659691612	24.492943839
O	1.583782914	3.176086690	24.301320413
H	1.658659373	2.221440270	24.022565390
H	1.179976700	3.166335846	25.194770981
O	3.483238797	8.200661289	14.893171560
H	3.853551035	7.378605552	15.419356771
H	3.485570159	7.939412382	13.949462144
O	2.191899690	-1.661201806	15.246885308
H	2.407976268	-2.596294407	15.298326564

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O        11.676416150   6.168172128  19.557632736
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H        11.469480128   5.306979737  19.092946104
O         8.117657181   8.401849210  23.455658748
H         8.181132671   8.766501581  22.547613953
H         7.497891335   7.631744076  23.431396981
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H         8.050455221  11.084509190  23.100755141
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H         5.009385950   3.579368716  14.279684527
H         6.033409843   2.490178613  13.706465827
O         1.502112255   1.769653776  15.280142743
H         1.737577991   1.597029357  16.233311859
H         0.556290541   2.035976729  15.143740205
O         4.348613725   4.700451764  18.532175086
H         5.253040351   4.328077958  18.384836225
H         3.709313542   3.981664639  18.452588145
O        -0.417281022   1.470073310  18.818478406
H         0.243009986   2.150374628  19.064360182
H         0.035444648   0.719261867  18.506309424
O         8.451881697  -0.516697156  13.960826271
H         7.780160134  10.641618830  13.756829607
H         9.285429216  -0.833704047  14.293244132
O         8.093699101   2.540838444  17.183450757
H         7.216300102   2.205071176  16.974413729
H         8.635606561   1.868330080  17.689950332
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Initial coordinates of the $\sigma = +0.2\ e$ trajectory:

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Au        5.113345000   0.000000000   6.410460000
Au        7.670027730   1.476096250   6.410460000
Au        5.113345000   2.952192500   6.410460000
Au        7.670027730   4.428288750   6.410460000
Au        5.113345000   5.904385000   6.410460000
Au        7.670027730   7.380481250   6.410460000
Au        5.113345000   8.856577500   6.410460000
Au        7.670027730  10.332673750   6.410460000
Au        0.000000000   0.000000000   6.410460000
Au        2.556672500   1.476096250   6.410460000
Au        0.000000000   2.952192500   6.410460000
Au        2.556672500   4.428288750   6.410460000
Au        0.000000000   5.904385000   6.410460000
Au        2.556672500   7.380481250   6.410460000
Au        0.000000000   8.856577500   6.410460000
Au        2.556672500  10.332673750   6.410460000
Au        6.817796740   0.000000000   8.820910000
Au        9.374469240   1.476096250   8.820910000
Au        6.817796740   2.952192500   8.820910000
Au        9.374469240   4.428288750   8.820910000
Au        6.817796740   5.904385000   8.820910000
Au        9.374469240   7.380481250   8.820910000
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Au	6.817796740	8.856577500	8.820910000
Au	9.374469240	10.332673750	8.820910000
Au	1.704451740	0.000000000	8.820910000
Au	4.261124240	1.476096250	8.820910000
Au	1.704451740	2.952192500	8.820910000
Au	4.261124240	4.428288750	8.820910000
Au	1.704451740	5.904385000	8.820910000
Au	4.261124240	7.380481250	8.820910000
Au	1.704451740	8.856577500	8.820910000
Au	4.261124240	10.332673750	8.820910000
Au	8.522248480	0.000000000	11.231400000
Au	5.965575980	1.476096250	11.231400000
Au	8.522248480	2.952192500	11.231400000
Au	5.965575980	4.428288750	11.231400000
Au	8.522248480	5.904385000	11.231400000
Au	5.965575980	7.380481250	11.231400000
Au	8.522248480	8.856577500	11.231400000
Au	5.965575980	10.332673750	11.231400000
Au	3.408903480	0.000000000	11.231400000
Au	0.852224850	1.476096250	11.231400000
Au	3.408903480	2.952192500	11.231400000
Au	0.852224850	4.428288750	11.231400000
Au	3.408903480	5.904385000	11.231400000
Au	0.852224850	7.380481250	11.231400000
Au	3.408903480	8.856577500	11.231400000
Au	0.852224850	10.332673750	11.231400000
O	3.174407839	8.885569710	23.565253910
H	3.342207432	7.952912601	23.744873124
H	2.850875803	9.219891126	24.416345793
O	4.045390418	4.564254159	20.901614730
H	3.254557215	4.024715490	21.053039948
H	4.690035360	3.890822822	20.580989701
O	2.925694174	8.619463630	17.327172869
H	3.361680847	7.745339415	17.481433402
H	2.275273492	8.522864611	16.584907151
O	0.019128389	4.221716935	21.156563057
H	0.351771044	3.673066368	21.923824640
H	0.410792674	3.833135653	20.365612681
O	1.977407831	9.134484178	21.143035037
H	2.587030188	8.499260820	20.703324062
H	2.277561138	9.104801876	22.089138368
O	3.824997750	7.569418352	14.500374096
H	3.974948611	6.849644564	15.155430001
H	3.702137537	7.077223995	13.668288046
O	6.515683450	0.370385412	23.677411977
H	5.529169664	0.364406763	23.626353581
H	6.764180066	11.498704418	24.317034866
O	4.310563661	-0.157887890	20.262897573
H	4.759966008	10.996012409	20.834120226
H	4.344954581	11.167912986	19.398795031
O	7.528682452	1.021536352	21.137073918
H	7.490419261	12.050235265	20.549904112
H	7.269166112	0.662435834	22.013510412
O	9.673971258	10.848214868	17.532034007

H	9.321925818	9.945077558	17.607073582
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H	7.492112243	2.674184164	14.255682290
H	6.043641529	3.125019791	14.167297053
O	1.335704574	6.009769557	17.718789636
H	1.431659097	5.021391939	17.854036583
H	1.816532170	6.213858472	16.904873543
O	6.838267138	5.575973705	18.515721058
H	6.942084913	5.178034809	19.411143054
H	7.527098838	5.097472171	18.003501160
O	1.288611507	0.190984759	21.713665125
H	1.934924645	11.297457571	21.536900709
H	0.443725847	11.468483782	21.901114110
O	5.585084079	2.411641637	19.932470532
H	6.443895241	2.114616269	20.339944403
H	5.106228313	1.554559036	19.919411764
O	0.019346633	11.582864213	15.070027473
H	9.903388411	10.845021815	14.519107445
H	10.082371459	11.277372638	16.009421132
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H	4.675640644	4.860097692	23.906068264
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H	9.102884338	4.678840885	16.103804463
H	9.082638829	4.351941626	14.626945630
O	7.581404963	4.592699974	21.011307029
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H	7.255621589	3.890792312	21.596221293
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H	9.282095786	9.789102161	22.622029647
O	9.816906301	2.518210398	14.492927706
H	9.754412126	2.130077612	13.599149109
H	9.589143596	1.775713901	15.080089687
O	8.269797391	1.498805887	18.115317078
H	8.803790824	0.697431404	17.956553325
H	7.335577597	1.207934201	17.949628501
O	8.700277747	9.681798407	13.735487521
H	7.736752368	9.757506527	13.587805542
H	8.745984777	8.828006235	14.258965707
O	1.749611932	10.582472458	18.747810174
H	2.076823947	9.758712879	18.300626197
H	1.758904114	10.367762921	19.709599186
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H	7.914841253	7.785865214	22.767032160
H	9.299424739	7.757277016	22.120336391
O	7.032195474	8.308273733	17.998367847
H	6.746606483	7.419881134	18.307229576
H	8.030252232	8.168247536	17.977772780
O	1.048515637	8.638291708	15.400872936
H	1.232941708	7.862246854	14.806422002
H	0.132835201	8.450380366	15.687744215
O	10.163033710	7.118710243	20.718058394

H	0.792456873	7.589025151	20.861249102
H	0.129096716	6.160232316	20.767730951
O	5.332783408	11.102276394	14.901001969
H	5.812094317	10.250295400	14.787792166
H	4.380664269	10.838330133	14.852984648
O	7.207214834	2.965356359	23.744907436
H	7.973861128	3.056170024	24.327539937
H	6.935164673	2.012627150	23.804727148
O	4.870470756	10.190112669	18.042712518
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H	4.124986850	9.708303115	17.600159199
O	4.687032156	3.414827361	17.369065580
H	4.763263912	2.530717928	16.965690211
H	5.191545849	3.308658599	18.202599794
O	1.173927458	6.321231247	14.217037180
H	0.452528775	5.761829214	14.609881099
H	1.685054765	5.764407284	13.602147959
O	8.684119020	7.665035624	15.386705986
H	7.819371468	7.768017371	15.819566810
H	8.753705515	6.692633940	15.184828295
O	10.152413133	5.588666682	24.113170035
H	10.172560066	4.655167304	24.333566837
H	9.767236946	5.656858766	23.226861624
O	2.185802519	1.051385528	17.132638144
H	2.463458597	0.768018900	16.247393621
H	2.102338116	12.066835913	17.703563082
O	6.168796242	8.696546776	14.076367758
H	6.610766963	7.808600023	14.102321176
H	5.232799715	8.380120945	14.220661865
O	2.319047149	2.232903354	20.281880578
H	1.768097850	1.539960367	20.732089648
H	3.103999821	1.742540635	19.979218572
O	4.727049532	2.027895630	14.656006505
H	5.010209612	1.097311886	14.738095452
H	3.761894766	1.945450794	14.545021848
O	5.840259714	0.779399620	17.254931795
H	6.167467450	12.379924164	16.362118609
H	5.451400759	11.719201399	17.527330007
O	3.963833758	0.763463592	23.108586635
H	3.124950690	0.474596689	23.490242681
H	3.863836958	0.670892632	22.146349796
O	4.205301977	4.843716105	14.910043337
H	4.530704023	4.321237468	15.671002632
H	3.445303384	4.326797821	14.556975186
O	2.855596229	6.849044051	20.020995751
H	2.349794306	6.649682345	19.207815158
H	3.447633355	6.070800583	20.167221264
O	5.282203406	9.293489016	21.700791721
H	4.675075344	9.358342664	22.467180818
H	5.602133253	8.356070092	21.729516780
O	1.137273384	2.655282159	23.145547520
H	1.199740104	1.754906854	22.757097210
H	0.734668599	2.489619210	24.008083335
O	2.902422400	10.205364531	14.382547280

H	2.085426450	9.916841148	14.856534585
H	3.260869839	9.343209218	14.104171444
O	2.234920775	0.936320420	14.165433049
H	2.630877202	0.141210970	13.755518748
H	1.357960492	0.569134764	14.471250248
O	9.593308438	8.017837165	18.176386637
H	9.708744776	7.798431687	19.136252475
H	10.070076441	7.282379491	17.737738232
O	6.472405722	6.865460445	22.145999655
H	6.899099041	6.194612445	21.559801147
H	6.069810039	6.279723308	22.850799136
O	7.473626534	10.130997626	20.239289582
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H	7.342728145	9.496776528	19.501828813
O	6.548868916	6.117324732	14.322970399
H	5.647139533	5.728490780	14.382762585
H	7.106573141	5.313097508	14.303448799
O	1.960248587	3.615905060	13.952074884
H	2.152862980	2.732160768	13.573850454
H	1.126079351	3.406397594	14.443737805
O	4.346584454	6.221185919	17.381179176
H	5.246180379	6.103603417	17.762884173
H	4.049445183	5.292275210	17.334199374
O	1.322322054	3.403345177	18.113287129
H	1.749843139	3.032514142	18.931316502
H	1.561236445	2.667694681	17.495510651
O	7.606676784	0.712975915	14.389635245
H	8.271482912	11.860488949	14.644089473
H	6.784303937	0.210962856	14.238455783
O	8.896048206	3.927752031	17.529061154
H	8.569854322	2.970824793	17.614955795
H	9.820414455	3.858285176	17.863712422

Initial coordinates of the $\sigma = +0.4\ e$ trajectory:

Au	5.799776829	−0.158542157	6.410460017
Au	8.484172050	1.407882777	6.410460017
Au	6.122186702	2.926058435	6.410460017
Au	8.573677987	4.576814038	6.410460017
Au	6.122546608	6.073008003	6.410460017
Au	8.656684160	7.482968567	6.410460017
Au	6.260444383	8.884357166	6.410460017
Au	8.782948805	10.384701912	6.410460017
Au	0.864699091	0.229869785	6.410460017
Au	3.518459656	1.667466093	6.410460017
Au	0.898062719	3.076684134	6.410460017
Au	3.628981003	4.563718576	6.410460017
Au	1.102728579	5.920500511	6.410460017
Au	3.839037014	7.640788576	6.410460017
Au	1.000347462	8.696670428	6.410460017
Au	3.249749737	10.633727989	6.410460017
Au	8.142020248	−0.054556550	8.965861111
Au	10.575515669	1.624901402	9.026385755

Au	7.913313523	2.909946746	9.059004516
Au	10.090753067	4.672257774	8.843276392
Au	7.622076871	5.824733553	8.786813322
Au	10.491872802	7.595476248	8.990134219
Au	7.928759140	8.915124688	8.927166991
Au	10.591282129	10.283552926	8.797772881
Au	2.862533729	0.216037557	8.933880567
Au	5.418968532	1.426741492	9.124962144
Au	2.337246418	3.259453982	8.933724942
Au	5.035318191	4.329954498	8.894472921
Au	2.834098834	6.134843839	8.881573004
Au	5.401268885	7.509696109	8.962480654
Au	2.832263932	9.124895738	9.098708622
Au	5.298765450	10.335614811	8.810888419
Au	9.728466898	0.071866192	11.431029755
Au	6.675029246	1.875058290	11.557551471
Au	9.784118388	3.117898406	11.320144174
Au	7.157275295	4.551286016	11.827056979
Au	9.618127078	6.184731482	11.475463026
Au	7.149007869	7.540630506	11.226378753
Au	9.689022826	9.042710609	11.519900955
Au	7.269678541	10.326953997	11.542049665
Au	4.621129224	-0.146224698	11.433997647
Au	1.883226656	1.510450848	11.432205258
Au	4.172652600	3.250950344	11.367747486
Au	1.830909190	4.612753625	11.301114187
Au	4.535871582	5.974348075	11.178067009
Au	1.958505324	7.457927486	11.573132815
Au	4.632188918	8.963142798	11.578654018
Au	2.012425723	10.557902512	11.603628869
O	1.909546471	9.460504051	22.144395451
H	1.501061692	9.467645863	23.115328772
H	2.763831335	9.986823442	22.177953399
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H	3.478936087	2.386680009	17.745916436
O	1.262437898	6.116699576	17.924868379
H	0.524282468	5.881252683	18.615510426
H	1.193124902	5.263765450	17.332392940
O	-5.687484221	1.355968333	26.000832219
H	-5.508168764	1.403312599	26.917924249
H	-5.896929949	0.433013434	25.999244602
O	7.229642090	7.683588593	20.893980453
H	7.940799740	7.046263729	21.302157794
H	7.789487953	8.358162473	20.442284060
O	2.463193876	5.353481519	14.065129248
H	2.851440983	5.172361625	14.949609685
H	2.924692113	4.710278248	13.537664158
O	5.901669303	2.037906900	20.934024173
H	4.987723797	1.779155106	21.023401674
H	6.495688620	13.223541711	20.684282959
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H	4.998362463	10.418970972	20.257279401
H	5.430316184	10.508897084	18.737143623

O	9.181151475	-0.934041110	25.240579928
H	9.383754206	11.697446116	25.667972626
H	8.271202197	-0.899041601	24.904799833
O	10.541375249	8.568836588	16.966303289
H	11.051142252	7.750507419	17.329526846
H	11.212546304	9.248711067	16.899541435
O	6.571645188	1.766648649	13.779302649
H	7.018727165	0.962117313	14.065310897
H	5.650951453	1.916976121	14.162006540
O	1.955498796	3.788260547	20.200039811
H	2.386715967	3.587138569	19.315216612
H	1.630904938	2.941165938	20.467414165
O	5.989188425	3.541113866	18.424564310
H	6.155976341	4.468091832	18.559306487
H	5.944971630	3.239721239	19.404495698
O	0.911073238	-1.104803402	19.519374445
H	1.404290221	10.572894558	18.692658783
H	0.954849217	9.990682761	20.184418047
O	4.317263222	0.912375909	17.708459151
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H	10.066258329	8.635539967	15.358953532
H	9.063124466	8.643920594	14.072093830
O	0.926726310	9.304234589	24.543496710
H	0.130446551	9.833896742	24.854225296
H	1.746790470	9.491957786	25.105295177
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H	6.016070566	4.406039376	23.064927509
H	6.535099630	3.175423363	22.190310765
O	9.967109682	2.055510707	22.895550230
H	10.724412112	1.973749039	23.515972553
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O	9.403331882	2.940393554	14.435651355
H	8.523018873	3.314352714	14.870205918
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O	6.201420155	-2.033425809	17.320280697
H	7.008346475	-2.155322261	17.883229453
H	6.511097726	-1.988074197	16.379823722
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H	4.620421846	12.182695464	14.566758515
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H	3.237925314	7.888293020	19.164862727
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O	16.861553888	9.767756195	23.557492063
H	17.482423825	9.085089920	23.317947024
H	16.577716075	9.521392039	24.447119144
O	6.768598981	6.416790851	18.612802678
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H	6.947151543	6.753200499	19.629224014

O	-1.585561113	3.158845668	18.433572429
H	-2.558494554	3.311655715	18.273362843
H	-1.258382003	3.905325963	18.967712818
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O	7.542082830	7.659051858	14.404779057
H	7.901489447	7.134416205	15.162815644
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H	-2.752413243	7.956948830	26.914542491
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H	3.732665278	6.432053258	20.336199456
O	1.920305353	-0.704254986	17.027270790
H	1.984015140	-0.948143384	16.090499931
H	2.802296179	-0.390191127	17.280968285
O	-0.375523652	5.696852689	14.050260992
H	0.649526806	5.490215361	14.024470018
H	-0.704250618	4.790750728	14.006653426
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H	10.220626360	7.724937812	24.398617894
H	8.908460030	7.235034475	25.056531690
O	-0.617709694	-0.058570501	16.655531146
H	-0.920818771	-0.103277054	17.607061179
H	0.389400819	11.695900913	16.743530245
O	5.648419960	5.554801358	14.161474910
H	5.178619099	5.064513914	13.447277126
H	5.151964480	5.307626923	14.950970420
O	1.028908910	1.291336105	20.703641046
H	1.057291957	0.447048716	20.243375465
H	0.354972316	1.402531344	21.456587964
O	6.449369580	-1.999625581	14.891145381
H	7.098785422	-1.480270014	14.436557353
H	6.723871791	-2.878375121	14.514110014
O	4.401081219	-3.997071140	16.931085035
H	5.289300757	8.167552462	17.111748590
H	3.796502504	8.247094166	17.612420252
O	3.464531156	0.869082768	21.730055291
H	2.622020408	0.994149316	21.220280768
H	3.595027049	-0.062328712	21.907050347
O	0.548150281	3.420956710	17.067049325
H	0.434923846	3.179088796	16.096436753
H	-0.448925924	3.215829481	17.418988610
O	4.263052688	5.977379291	24.440347261
H	3.870542994	6.302866692	25.296969255
H	3.592825393	6.159234338	23.777820867
O	5.007086474	9.141153417	21.415231391
H	5.429645590	9.429544331	22.288945051
H	5.537811926	8.294622988	21.303013084

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O         2.225255073  14.119590449  24.323560822
H         2.485838868  14.216041107  25.237994660
H         3.052654049  13.855202467  23.901044751
O         3.522899503   8.065144392  14.228839163
H         3.312278096   7.135390873  14.144880394
H         3.894185038   8.109162891  15.148819720
O         1.584601002  -1.071015643  14.294813188
H         2.521456718  -1.342822957  14.262015850
H         0.966632469  -1.922132349  14.187397816
O         9.844710385   5.157627059  19.871117817
H        10.604686165   4.631188167  20.089361364
H         9.537728051   5.414640546  20.846116620
O         8.825594199   5.889443473  22.174617746
H         8.079575087   5.337981690  22.573787062
H         9.252103167   6.267052686  22.990503811
O         8.460118137   9.282313027  18.882494119
H         9.086779357   8.990155343  18.124562905
H         8.782744462  10.169341762  19.129758787
O         4.305094766   2.534825783  14.605661928
H         4.517719176   2.978383904  15.412873030
H         3.320463449   2.325303169  14.666391585
O         1.780061405   1.901858011  14.685253196
H         1.533489084   0.914430427  14.439077632
H         1.023403593   2.400460676  14.296984695
O         4.371153760   5.209470931  16.371887133
H         4.120501764   4.491390303  17.058034444
H         4.358809026   6.146776997  16.730594922
O        -2.082634838   0.402055252  19.639166176
H        -2.563229876   0.423051891  18.730847620
H        -1.565066827   1.275913770  19.601707818
O         8.249380106  -0.006051649  14.454700058
H         8.832846232  11.630028458  15.291841072
H         8.829576329  -0.336392414  13.720721498
O         6.997654529   0.939178981  17.210478136
H         6.753458973   1.851004606  17.262580117
H         7.746478110   1.025358374  16.519101143
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