

Photo-oxidation Mechanism of Water on $\text{WO}_3(001)$ - A combined Embedded Cluster, Machine Learning and Wave Packet Approach

T. Teusch, T. Klüner

Carl von Ossietzky University, Oldenburg, Germany

S1 Supporting Information

S1.1 Basis set

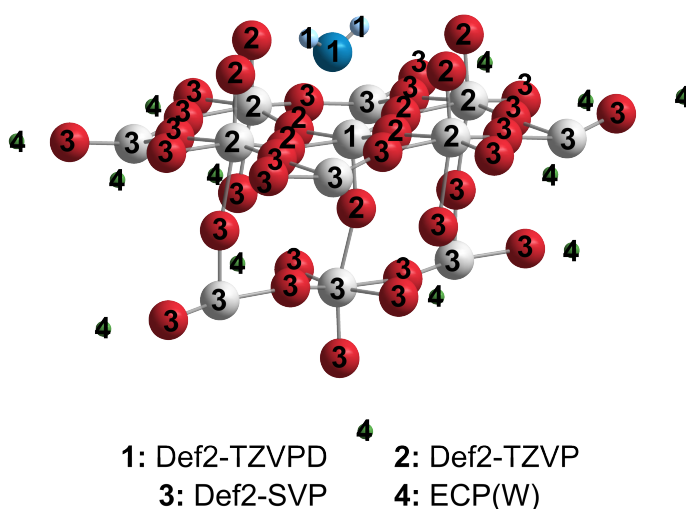


Figure S1: Assignment of the different basis sets on each atom within the cluster model.

S1.2 Grid for each jacobian coordinate

Table S1: Grid for each jacobian coordinate.

Jacobian Coordinate	Value range
$\vartheta / ^\circ$	0, 24, 48, 54.54, 72, 96, 120, 144, 168, 180
Y / Å	-3.49, -3.39, -3.28, -3.18, -3.07, -2.91, -2.75, -2.59, -2.43, -2.28, -2.12, -1.96, -1.80, -1.64, -1.48, -1.32, -1.16, -1.01, -0.85, -0.69, -0.53, -0.37, -0.21, -0.05, 0.11, 0.26, 0.42, 0.58, 0.74, 0.90, 1.06, 1.22, 1.38, 1.53 + specific points
Z / Å	18.52, 13.23, 7.94, 6.35, 5.29, 5.03, 4.76, 4.50, 4.23, 3.97, 3.70, 3.44, 3.18, 2.91, 2.65, 2.38, 2.28, 2.17, 2.06, 1.96, 1.85, 1.75, 1.64, 1.53, 1.32 + specific points

S1.3 Cluster size convergence

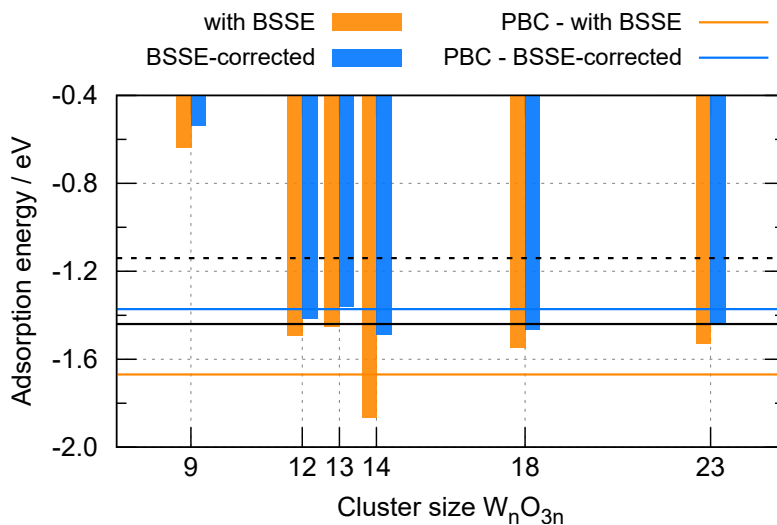


Figure S2: Convergence of the cluster size with respect to periodic boundary calculations (PBC) including the BSSE using PBE0.

S1.4 Different structures of the neural networks

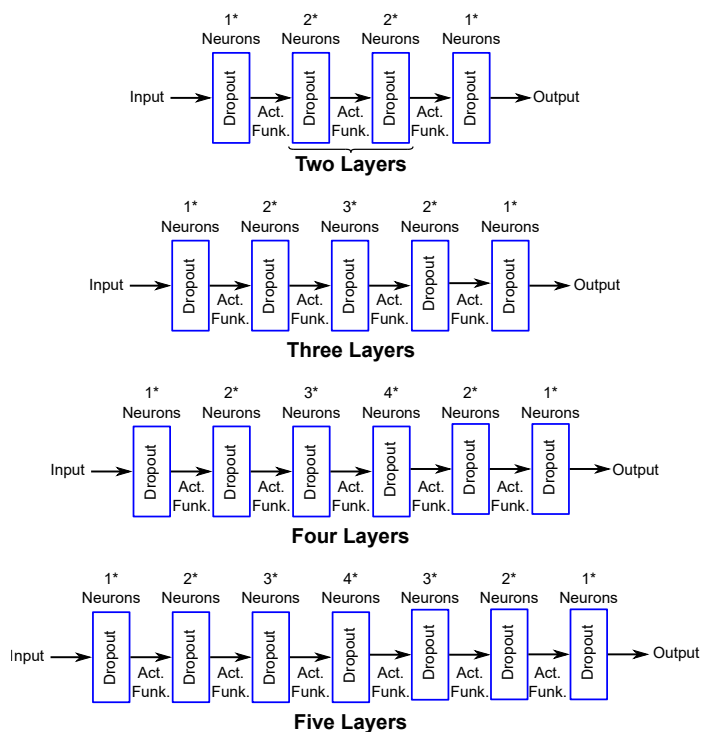


Figure S3: Structure of the neural networks in terms of layers and neurons.

S1.5 Activation functions

Table S2: Different activation functions σ including value range.

Name	Activation Function	Value Range
ReLU	$\sigma(x) = \begin{cases} x & \text{für } x \geq 0 \\ 0 & \text{sonst} \end{cases}$	$[0, \infty]$
Leaky ReLU	$\sigma(x) = \begin{cases} x & \text{für } x > 0 \\ 0.01 \cdot x & \text{sonst} \end{cases}$	$[-\infty, \infty]$
Rand. ReLU	$\sigma(x) = \begin{cases} x & \text{für } x > 0 \\ a \cdot x & \text{sonst} \end{cases}$	$[-\infty, \infty]$
SELU	$\sigma(x) = \lambda \begin{cases} x & \text{für } x > 0 \\ \alpha \cdot \exp(x) - \alpha & \text{sonst} \end{cases}$	$[-\alpha \cdot \lambda, \infty]$
CELU	$\sigma(x) = \begin{cases} x & \text{für } x \geq 0 \\ a \left(\exp\left(\frac{x}{a}\right) - 1 \right) & \text{sonst} \end{cases}$	$[a, \infty]$
tanh	$\sigma(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$	$[-1, 1]$
Sigmoid	$\sigma(x) = \frac{1}{1 + \exp(-x)}$	$[0, 1]$
Tanhshrink	$\sigma(x) = x - \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$	$[-\infty, \infty]$

Randomized ReLU: a is a random number between $\frac{1}{8}$ and $\frac{1}{3}$
 SELU: $\alpha = 1.6732632423543772848170429916717$
 $\lambda = 1.0507009873554804934193349852946$
 CELU: $a = 1$

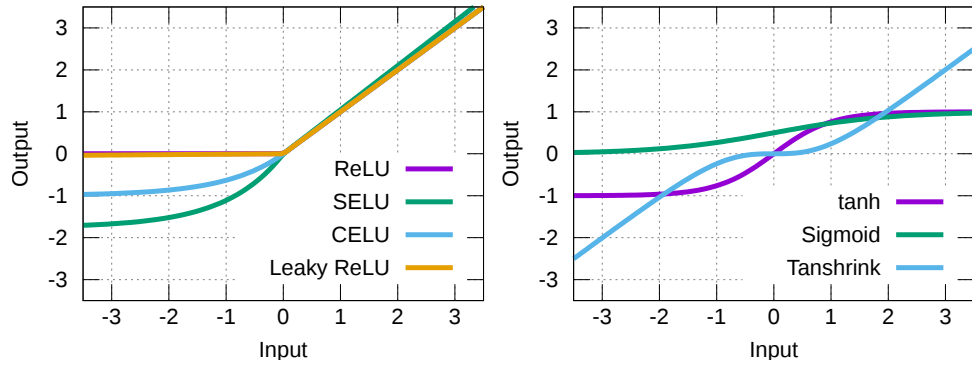


Figure S4: Visualisation of the *linear unit* activation functions (left) and classical functions (right).

S1.6 (2+2)-Genetic Algorithm Pseudocode

Algorithm 1 (2+2)-Genetic Algorithm

```

procedure (2+2)-GA
  Initialize two random parents
  Calculate fitness of both parents
  for  $i = 0, 99$  do
    Crossover
    Mutation
    Neural Network Fits
    parents  $\leftarrow$  best two solutions
  end for
  return best solution
end procedure

```

\triangleright 100 iterations \rightarrow 200 nets \rightarrow 1/5 of all data
 \triangleright Recombination of bitstrings
 \triangleright Using Rechenberg 1/5 rule

S1.7 Wave packet dynamics and photodesorption

We have used the split propagator throughout. Formulated in real time the following expression results:

$$\exp(-i\hat{H}\Delta t) \approx \exp\left(-i\frac{\hat{T}}{2}\Delta t\right) \cdot \exp(-i\hat{V}\Delta t) \cdot \exp\left(-i\frac{\hat{T}}{2}\Delta t\right) \quad (\text{S.1})$$

In imaginary time we substitute the time t with the imaginary time $\tau = i \cdot t$ resulting in

$$\exp(-\hat{H}\tau) \approx \exp\left(-\frac{\hat{T}}{2}\tau\right) \cdot \exp(-\hat{V}\tau) \cdot \exp\left(-\frac{\hat{T}}{2}\tau\right) \quad (\text{S.2})$$

Due to the exponent term, all summands are now striving towards 0 if the propagation time is sufficiently long. Since the ground state wave function is energetically lowest, this state remains longest. The simulation of the photodesorption process is depicted in figure S5 with different residence lifetimes τ_n .

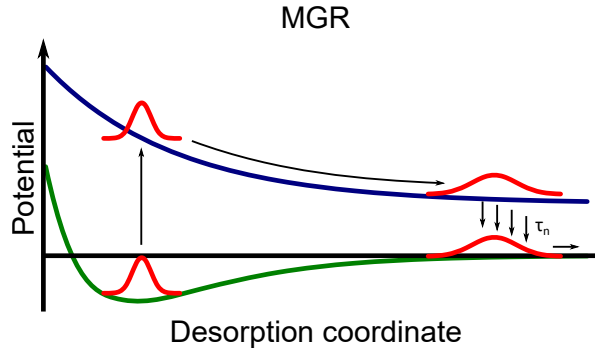


Figure S5: Menzel-Gomer-Redhead (MGR) mechanism of the photodesorption process [1,2].

The wave packet is generated on the ground state (green potential) by imaginary time propagation and then vertical transferred to the CT state (blue potential). The wave packet is then propagated on the CT state in real time. We performed the *jumping wave packet method* to relax the wave packet back on the ground state after selected time steps and propagated it there until convergence of the expectation values. It has been shown that this procedure is equivalent to a solution of the Liouville-Neumann equation for open quantum systems [3]. Although this jumping wave packet scenario is a simple way to treat electronic relaxation, it has been shown that this stochastic approach gives almost identical results to the Surrogate Hamiltonian method which treats the whole photodesorption scenario, including electronic relaxation, in a much more sophisticated model from first principles [4].

[1] D. Menzel, R. Gomer, *J. Chem. Phys.* **1964**, 41, 3311.

[2] P. A. Redhead, *Can. J. Phys.* **1964**, 42, 886.

[3] P. Saalfrank, *Chem. Rev.* **2006**, 106, 4116-4159.

[4] S. Dittrich, H.-J. Freund, *et al.*, *J. Chem. Phys.*, **2006**, 124, 024702.

S1.8 Genetic algorithm

Table S3: Hyperparameter combination considered by genetic algorithm for ground state PES fitting. The optimized combination is highlighted in bold.

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
4	32	CELU	MAE	0.00	0.017873940	0.016732890
5	32	CELU	LogCosh	0.01	0.096470690	0.099655200
4	128	Tanhshrink	MSE	0.00	1.774340880	1.718528190
2	128	Sigmoid	LogCosh	0.00	0.020286140	0.023106120
4	128	Sigmoid	MSE	0.00	0.020844190	0.045571210
4	32	Sigmoid	LogCosh	0.00	0.010792230	0.016261950
4	32	RReLU	LogCosh	0.00	9.999999998	9.999999998
4	128	Sigmoid	MAE	0.00	1.704198220	1.554776350
4	64	Sigmoid	LogCosh	0.00	1.598240250	1.683007440
4	128	Sigmoid	MSE	0.01	1.755993410	1.805787220
2	128	SELU	LogCosh	0.00	0.013468970	0.037764470
4	32	Sigmoid	LogCosh	0.05	1.682656450	1.697179520
4	256	Tanh	LogCosh	0.00	0.019406830	0.019747230
4	128	Sigmoid	MSE	0.05	1.796478800	1.623941730
4	32	Sigmoid	MSE	0.00	0.022230240	0.021280700
5	32	Tanh	LogCosh	0.01	0.269033980	0.228581830
4	128	Sigmoid	MSE+MAE	0.00	1.667948940	1.716534210
4	64	Sigmoid	MSE	0.00	0.007566390	0.014550040
4	128	Sigmoid	LogCosh	0.00	0.020616400	0.026438220
4	32	Tanhshrink	MSE	0.00	1.774589420	1.710616890
5	32	Sigmoid	MSE	0.00	1.758427290	1.786320520
4	256	Tanhshrink	MSE	0.00	1.750049950	1.835602380
4	128	Sigmoid	LogCosh	0.01	1.669700450	1.769719780
4	32	Sigmoid	MSE	0.05	1.776334110	1.724681240
4	64	Tanhshrink	MAE	0.00	1.694207180	1.617423710
2	32	Sigmoid	LogCosh	0.00	0.024996180	0.027107180
4	128	Tanh	MSE	0.00	0.024568360	0.037682790
4	32	Tanhshrink	LogCosh	0.00	1.687917670	1.672836210
4	256	Sigmoid	LogCosh	0.00	0.004258620	0.035270360
4	32	Sigmoid	MSE	0.01	1.747923730	1.836292960
5	128	Tanhshrink	MSE+MAE	0.00	1.666618040	1.723708080
2	128	Sigmoid	MSE	0.00	0.017766990	0.031180350
4	128	CELU	MSE	0.01	0.022657550	0.032512820
4	32	RReLU	LogCosh	0.01	0.494666540	0.509735460
5	128	Sigmoid	LogCosh	0.00	1.681096500	1.703693440
4	32	Tanhshrink	MSE	0.01	1.785443780	1.681737100
4	128	Tanhshrink	LogCosh	0.00	1.670188290	1.773468280
5	32	Sigmoid	LogCosh	0.00	1.672052480	1.752041210

Continued on next page

Table S3 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
4	128	Tanhshrink	MSE	0.05	1.753234940	1.823089580
4	64	RReLU	LogCosh	0.00	0.237800870	0.256689120
5	128	Tanh	LogCosh	0.00	0.020699000	0.020230560
5	32	Tanhshrink	LogCosh	0.10	1.673412460	1.747944320
5	128	Sigmoid	LogCosh	0.01	1.683507800	1.693108780
4	32	Sigmoid	MAE	0.05	1.662528040	1.794000920
2	128	Sigmoid	MSE	0.01	0.028124220	0.045912000
2	32	RReLU	LogCosh	0.00	0.257997960	0.283363720
4	128	Tanh	LogCosh	0.00	0.021919690	0.026405260
4	32	Sigmoid	MAE	0.00	1.684486190	1.668871830
4	32	Sigmoid	LogCosh	0.01	1.690320040	1.660011370
4	128	RReLU	MSE	0.00	0.016395270	0.021749480
4	128	Tanhshrink	MSE+MAE	0.00	1.679926000	1.648536250
4	32	SELU	MSE	0.00	0.013967730	0.026142340
4	256	Sigmoid	MSE+MAE	0.00	0.005178120	0.017391240
2	32	Sigmoid	MSE	0.00	0.008365130	0.017093470
4	32	CELU	MSE	0.05	0.070272270	0.071368430
5	128	Sigmoid	MSE	0.00	1.752396790	1.837723370
5	128	Sigmoid	MSE+MAE	0.00	1.659298110	1.763318300
5	32	SELU	LogCosh	0.00	0.018800570	0.039248680
2	128	Tanh	LogCosh	0.00	0.006699160	0.021780620
5	32	Tanhshrink	MSE+MAE	0.00	1.688064200	1.601536430
5	32	RReLU	LogCosh	0.00	0.107862040	0.110441570
4	128	Tanhshrink	MSE	0.10	1.788527160	1.640843720
4	32	Tanh	LogCosh	0.10	0.144022350	0.150061070
4	32	Tanh	MSE	0.00	0.019103250	0.019943890
2	128	Tanhshrink	LogCosh	0.00	1.677701100	1.726911710
2	32	Sigmoid	MAE	0.05	0.366715560	0.387625260
4	128	RReLU	LogCosh	0.00	0.049110640	0.066576830
4	32	Sigmoid	MSE+MAE	0.00	1.660826160	1.755262820
4	128	Tanh	MSE	0.01	0.264646300	0.278177660
4	128	Sigmoid	LogCosh	0.05	1.692942920	1.639464320
4	32	SELU	LogCosh	0.00	0.007285040	0.041482030
5	128	Sigmoid	MAE	0.00	1.686018330	1.660201340
4	256	Sigmoid	MAE	0.00	1.685640970	1.663461610
4	32	CELU	LogCosh	0.00	0.007812140	0.018955230
2	256	Sigmoid	LogCosh	0.00	0.025238420	0.028205440
4	32	Tanh	LogCosh	0.00	0.018105930	0.020193300
4	128	RReLU	MSE+MAE	0.00	0.016189540	0.027736900
3	32	Sigmoid	MSE	0.00	0.015383960	0.030019270
2	128	Sigmoid	MSE	0.05	0.053454280	0.072648770

Continued on next page

Table S3 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
4	128	Tanhshrink	MSE	0.01	1.736200590	1.903448130
5	32	Tanh	LogCosh	0.00	0.009786260	0.017333240
4	128	Sigmoid	MSE	0.10	1.782420320	1.688238430
3	128	Tanh	LogCosh	0.00	0.019681050	0.023050570
4	256	Sigmoid	MSE	0.00	0.005654550	0.033978340
5	128	Tanhshrink	LogCosh	0.05	1.661089830	1.814585080
4	32	RReLU	MSE	0.00	0.030259660	0.035595240
2	128	Sigmoid	MSE+MAE	0.00	0.012905400	0.038525240
2	32	Tanh	MSE	0.00	0.022240540	0.025888510
5	32	RReLU	MSE	0.00	0.023223020	0.028626730
4	32	Tanh	MAE	0.00	0.019170070	0.018574000
5	128	Tanh	MSE	0.05	0.037658550	0.056033530
4	32	Sigmoid	MSE+MAE	0.01	1.684758220	1.621099920
4	128	Tanh	MSE	0.05	0.086547990	0.095958680
4	64	Sigmoid	LogCosh	0.01	1.680455120	1.711761410
2	128	Sigmoid	LogCosh	0.05	0.036619930	0.055896600
4	32	Sigmoid	MSE	0.10	1.758294040	1.788704330
4	128	Sigmoid	LogCosh	0.10	1.671909690	1.756641040
4	32	RReLU	MAE	0.00	0.025616560	0.026778840
4	128	Leaky ReLU	LogCosh	0.01	0.162443490	0.190865180
4	32	RReLU	MSE	0.10	0.136877990	0.125148800
4	128	Tanhshrink	LogCosh	0.05	1.676132840	1.737408210
2	32	RReLU	MAE	0.00	0.050526070	0.059918050
5	128	RReLU	LogCosh	0.00	0.209022260	0.225961200
5	64	Sigmoid	MSE	0.00	1.744113080	1.858468680
5	128	Tanh	MSE	0.00	0.007452660	0.013695040
4	32	Tanhshrink	MSE+MAE	0.00	1.679982700	1.648201220
5	128	RReLU	MSE	0.00	0.030654930	0.037936360
5	32	Tanhshrink	LogCosh	0.05	1.675210090	1.737494330
4	64	Sigmoid	LogCosh	0.05	1.670747450	1.762110300
4	128	Leaky ReLU	MSE	0.00	0.002791920	0.034583760
4	32	Tanh	MSE+MAE	0.00	0.017553300	0.023245110
4	128	Leaky ReLU	MAE	0.00	0.014167490	0.031017770
4	256	Tanhshrink	LogCosh	0.00	1.679507350	1.715805380
4	32	Leaky ReLU	MAE	0.01	0.060354080	0.069510600
4	128	RReLU	MSE	0.01	0.027473870	0.032042650
4	32	Tanhshrink	MAE	0.00	1.679117940	1.704247060
5	256	RReLU	LogCosh	0.05	0.272794180	0.272489320
2	64	Sigmoid	MSE	0.00	0.021068600	0.018753470
4	128	Sigmoid	MSE+MAE	0.05	1.678837740	1.654789830

Continued on next page

Table S3 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
4	32	Tanhshrink	MAE	0.05	1.695330370	1.606960460
4	128	Tanhshrink	LogCosh	0.01	1.686086240	1.672591910
2	32	Sigmoid	MSE	0.05	0.103392430	0.113180100
2	128	Leaky ReLU	LogCosh	0.00	0.005257770	0.021702810
3	32	Sigmoid	MSE	0.01	0.131314050	0.133351980
2	256	Sigmoid	MSE	0.00	0.009428880	0.027547100
4	64	SELU	MSE	0.00	0.001528200	0.033251770
2	128	RReLU	MSE	0.00	0.024675890	0.031007690
4	64	Sigmoid	MSE+MAE	0.00	1.690151890	1.589561220
2	256	RReLU	MSE	0.00	0.019421610	0.029409320
4	32	Tanh	LogCosh	0.01	0.033777880	0.060709350
4	128	CELU	LogCosh	0.00	0.015892170	0.027540100
5	32	Sigmoid	MSE	0.01	1.786271450	1.667944500
4	128	RReLU	LogCosh	0.05	0.341414990	0.330105590
4	32	RReLU	LogCosh	0.05	0.627278630	0.603830950
2	32	Tanhshrink	LogCosh	0.00	1.677059400	1.730655120
4	128	Sigmoid	MAE	0.05	1.682310020	1.682645020
5	128	Sigmoid	MSE	0.01	1.771384550	1.724780460
4	256	Tanh	LogCosh	0.01	0.022221440	0.030305530
4	128	Tanhshrink	MAE	0.00	1.660332280	1.806320300
4	32	Tanhshrink	LogCosh	0.05	1.687550100	1.676459700
3	128	Sigmoid	LogCosh	0.00	0.020466930	0.025223220
4	32	CELU	MSE	0.00	0.004246830	0.029239300
4	256	Sigmoid	LogCosh	0.01	1.693979900	1.636313630
4	32	Leaky ReLU	MSE	0.00	0.002614590	0.024803230
5	128	Tanhshrink	LogCosh	0.00	1.687985480	1.666041710
5	32	Tanhshrink	MSE	0.00	1.759080650	1.796721500
4	256	RReLU	MSE	0.00	0.016097610	0.027471210
4	64	Tanhshrink	LogCosh	0.00	1.694711910	1.627393400
3	32	Sigmoid	LogCosh	0.00	0.013167950	0.036659990
4	128	RReLU	MSE	0.05	0.050613640	0.070971760
2	128	Tanh	MSE	0.00	0.019691210	0.024253740
4	64	Tanh	LogCosh	0.00	0.008948350	0.015898560
4	256	Sigmoid	LogCosh	0.05	1.681227820	1.711136660
2	32	Sigmoid	MSE	0.01	1.767986030	1.761272500
4	32	RReLU	MSE+MAE	0.00	0.024035800	0.031427270
4	256	Sigmoid	MSE	0.01	1.737500060	1.877924500
4	128	Tanh	MAE	0.00	0.015663010	0.026333000
2	32	Sigmoid	MSE+MAE	0.00	0.017442480	0.017413120
4	128	Tanh	MSE+MAE	0.00	0.002878690	0.021521460

Continued on next page

Table S3 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
5	32	Tanh	MSE	0.00	0.010018950	0.038573680
4	128	SELU	LogCosh	0.00	0.007916320	0.043688320
4	32	RReLU	MSE	0.05	0.111705740	0.114219410
5	32	Sigmoid	LogCosh	0.05	1.673497250	1.746972430
4	256	Tanh	MSE	0.00	0.015524150	0.021075360
4	128	RReLU	MAE	0.00	0.020133520	0.024820780
4	32	Tanh	LogCosh	0.05	0.101630160	0.116220050
2	128	RReLU	LogCosh	0.00	0.025853060	0.042362490
5	32	Sigmoid	MSE	0.05	1.771017460	1.739657950
4	128	Tanhshrink	MAE	0.01	1.687296150	1.654548620
5	128	Sigmoid	LogCosh	0.05	1.665028480	1.790090530
2	128	Tanhshrink	MSE	0.00	1.771969610	1.720501140
5	32	Tanhshrink	LogCosh	0.00	1.673650190	1.746709510
4	128	SELU	MSE	0.00	1.636436140	1.701639870
5	32	CELU	LogCosh	0.00	0.017048200	0.025277230
5	256	Sigmoid	LogCosh	0.00	1.688022920	1.673057430
4	64	RReLU	MSE	0.00	0.020421730	0.034689530
4	128	RReLU	LogCosh	0.01	0.774253750	0.816961190
4	64	Tanhshrink	MSE	0.00	1.760888650	1.791585530
4	256	Sigmoid	MAE	0.05	1.687815010	1.651619380
4	32	Tanh	MSE	0.05	0.105413990	0.111994450
4	256	Sigmoid	MSE	0.05	1.777869890	1.697559190
2	32	RReLU	MSE	0.00	0.043314580	0.057923910
4	32	Tanh	MSE+MAE	0.01	0.045857730	0.051231780
2	128	CELU	MSE	0.00	0.018974590	0.021096240
4	128	CELU	MSE	0.00	0.006337330	0.027822300
2	32	Tanh	LogCosh	0.00	0.025419660	0.027639920
2	128	Leaky ReLU	MSE	0.00	0.001057420	0.025369480
4	32	Tanhshrink	LogCosh	0.01	1.676656990	1.729960990
4	128	Sigmoid	MSE+MAE	0.01	1.682893570	1.630699370
4	64	Sigmoid	MSE	0.01	1.766514970	1.761998190
4	32	Sigmoid	LogCosh	0.10	1.680506660	1.707156690
3	128	Sigmoid	MSE	0.00	0.022977840	0.039231650
4	128	Sigmoid	MAE	0.01	1.687873330	1.652858090
2	32	Sigmoid	LogCosh	0.05	0.115389750	0.123467130
5	128	Tanhshrink	MAE	0.00	1.652195070	1.850433540
4	32	Tanh	MSE	0.01	0.100983570	0.111980900
3	128	Sigmoid	LogCosh	0.05	0.030027470	0.048608470
2	32	Sigmoid	MAE	0.00	0.019863380	0.020371050
2	128	Sigmoid	LogCosh	0.01	0.030873010	0.037223060
2	128	Sigmoid	MAE	0.00	0.014156520	0.045119440

Table S4: Hyperparameter combination considered by genetic algorithm for charge-transfer state PES fitting.

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
5	32	Sigmoid	MSE	0.10	2.800117890	2.833280430
4	256	RReLU	LogCosh	0.01	0.298483470	0.305868910
3	128	Tanhshrink	MAE	0.00	2.750994850	2.806069530
5	64	SELU	LogCosh	0.00	0.027651570	0.074822650
4	128	Leaky ReLU	MAE	0.00	0.030110410	0.045501800
5	256	Tanh	MSE+MAE	0.00	0.010890700	0.061954710
5	128	Sigmoid	LogCosh	0.00	0.038002800	0.045533820
5	256	ReLU	MAE	0.00	0.024422570	0.062487240
3	32	Sigmoid	LogCosh	0.05	0.809461090	0.808351100
5	256	Tanhshrink	MSE	0.00	2.812556570	2.782722510
5	128	Leaky ReLU	MAE	0.00	0.032262540	0.042871590
5	256	Tanh	LogCosh	0.00	0.036003860	0.075295040
3	256	ReLU	MAE	0.01	0.084392740	0.106259190
5	256	RReLU	LogCosh	0.01	1.561708690	1.539398000
5	128	SELU	MAE	0.01	0.042209300	0.085952170
5	64	Sigmoid	LogCosh	0.00	0.021603610	0.046658570
4	256	CELU	MSE	0.01	0.058107640	0.062303920
3	256	Sigmoid	LogCosh	0.00	0.004440480	0.034754120
5	128	Sigmoid	MSE+MAE	0.00	2.729687500	2.784535070
5	256	Leaky ReLU	MSE	0.00	0.023432750	0.065689490
5	128	Sigmoid	LogCosh	0.01	1.357632670	1.381425740
5	64	ReLU	MAE	0.00	0.037445190	0.048953510
5	128	Tanhshrink	MSE+MAE	0.00	9.508642790	9.486309410
5	256	SELU	LogCosh	0.00	0.032275210	0.059580380
5	64	SELU	MAE	0.00	0.041041300	0.073959620
5	128	Tanh	LogCosh	0.10	0.124677610	0.158724780
3	256	ReLU	MAE	0.00	0.029518630	0.046809410
4	128	Sigmoid	LogCosh	0.00	0.038203080	0.057428520
3	128	ReLU	MSE	0.01	0.079450620	0.091481250
3	256	Tanh	LogCosh	0.00	1.264314160	1.361305750
5	256	ReLU	MAE	0.05	0.116453370	0.149400070
5	256	Sigmoid	LogCosh	0.00	0.012975110	0.033025820
5	128	Sigmoid	MAE	0.00	2.799907810	2.496902420
5	256	ReLU	LogCosh	0.00	0.030003790	0.053801100
5	128	Tanhshrink	MAE	0.00	2.737570830	2.876153950
5	256	SELU	MSE+MAE	0.01	0.052005270	0.077625040
5	256	Leaky ReLU	MAE	0.00	0.032388090	0.064945070
5	128	Tanhshrink	MSE	0.00	2.802657700	2.829614910

Continued on next page

Table S4 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
4	256	ReLU	MAE	0.05	0.118878450	0.128731640
5	128	Sigmoid	MSE	0.05	0.087362630	0.120536870
5	128	Sigmoid	MSE+MAE	0.05	2.724721830	2.812461740
5	256	CELU	MAE	0.05	0.071096110	0.110773240
5	128	Sigmoid	MAE	0.01	2.743404970	2.837212640
5	256	SELU	MSE+MAE	0.00	0.030756500	0.054985130
5	128	Tanh	MSE+MAE	0.00	0.010046250	0.038485590
3	256	CELU	MSE	0.00	0.033379280	0.055676430
5	32	Sigmoid	MAE	0.00	2.777347180	2.639207550
4	128	SELU	MAE	0.00	0.029635830	0.075880030
5	256	ReLU	MSE	0.00	0.027993330	0.056534860
5	128	CELU	LogCosh	0.00	0.016275520	0.079819400
3	128	Tanh	MAE	0.05	0.149381430	0.188185460
5	64	Tanh	LogCosh	0.00	9.411213600	9.461619860
5	128	Tanh	LogCosh	0.00	0.031725060	0.035359110
5	256	SELU	MAE	0.01	0.049140570	0.087706800
5	256	ReLU	MSE+MAE	0.00	0.019288780	0.075782310
5	32	RReLU	LogCosh	0.00	0.749646370	0.710262370
5	128	Tanhshrink	LogCosh	0.00	9.999999998	9.999999998
5	256	ReLU	MAE	0.10	0.180228290	0.189577870
5	32	Sigmoid	LogCosh	0.00	0.027421340	0.059737240
4	256	Leaky ReLU	MAE	0.01	0.051000400	0.062476650
4	256	SELU	MAE	0.00	0.027966680	0.057656840
2	128	Sigmoid	LogCosh	0.00	9.999999998	9.999999998
4	128	Tanhshrink	MAE	0.00	2.750359970	2.799332130
4	256	SELU	LogCosh	0.00	0.027851020	0.061492360
5	64	RReLU	MAE	0.00	0.037715880	0.093066420
5	128	Sigmoid	MSE	0.00	0.003020520	0.023515760
5	128	CELU	MAE	0.00	0.032750630	0.057023490
5	256	Tanhshrink	LogCosh	0.00	2.715118160	2.903244150
5	256	CELU	MAE	0.00	0.035197000	0.036783460
5	32	ReLU	LogCosh	0.00	0.016311470	0.056226740
5	128	ReLU	MAE	0.00	0.028461660	0.050470450
4	256	Sigmoid	MSE	0.00	0.012368950	0.045999450
5	64	ReLU	MAE	0.01	0.085036040	0.108040410
3	128	Sigmoid	LogCosh	0.00	0.035524330	0.048147080
5	128	Leaky ReLU	MAE	0.05	0.152515850	0.171880750
2	256	ReLU	LogCosh	0.00	0.027761830	0.048314820
5	128	RReLU	MAE	0.01	0.058871470	0.102580750
5	256	CELU	LogCosh	0.00	0.039133650	0.064054750
5	256	ReLU	MAE	0.01	0.058166340	0.069183830

Continued on next page

Table S4 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
4	128	Sigmoid	MSE+MAE	0.00	0.023730000	0.045198590
5	128	Sigmoid	LogCosh	0.05	1.301203530	1.249895500
5	128	ReLU	MSE+MAE	0.01	0.057478200	0.073299000
4	32	Tanhshrink	MSE+MAE	0.00	2.742995820	2.709249340
5	256	ReLU	MSE	0.05	0.116400780	0.124122120
5	128	SELU	MAE	0.00	0.030746500	0.074738750
3	64	Sigmoid	LogCosh	0.00	0.020373380	0.045923580
5	256	ReLU	MSE+MAE	0.05	0.101661290	0.119989750
3	128	Tanh	LogCosh	0.00	0.044501550	0.059351810
4	128	ReLU	MSE+MAE	0.01	0.049824090	0.099925220
2	128	Sigmoid	LogCosh	0.05	0.067466030	0.117317150
3	128	Leaky ReLU	MAE	0.00	0.028185230	0.056636470
5	256	CELU	MSE+MAE	0.00	0.030702600	0.056063350
4	256	Sigmoid	LogCosh	0.05	0.068316250	0.111489350
5	256	SELU	MAE	0.00	0.040723950	0.056615400
5	128	ReLU	MAE	0.01	0.061924680	0.078998430
5	256	Sigmoid	MSE	0.00	0.135106940	0.273388920
4	256	Sigmoid	MSE+MAE	0.00	0.005751780	0.026277870
5	64	ReLU	MSE	0.00	0.030702310	0.076643920
5	128	Tanhshrink	MAE	0.05	2.750665850	2.827409390
5	256	SELU	MSE	0.05	0.280687190	0.273095780
2	128	Sigmoid	LogCosh	0.01	9.999999999	9.999999999
4	256	Leaky ReLU	MAE	0.00	0.028952410	0.050747500
5	128	RReLU	LogCosh	0.00	0.050609220	0.078246050
5	256	ReLU	MSE	0.01	0.044989890	0.069609230
3	128	ReLU	MAE	0.01	0.067439040	0.078800290
5	256	Sigmoid	LogCosh	0.01	9.999999999	9.999999999
5	256	Tanhshrink	MAE	0.00	2.757349740	2.762861930
4	128	Sigmoid	MSE	0.00	0.030854010	0.071289500
5	128	Leaky ReLU	MSE	0.00	0.001828990	0.068159130
5	256	Sigmoid	MSE+MAE	0.00	0.010103620	0.036983020
5	256	ReLU	MSE+MAE	0.01	0.048510050	0.056458000
5	128	RReLU	MSE	0.00	0.039081270	0.050144280
5	128	CELU	MSE	0.05	0.086102810	0.120318060
5	256	SELU	MSE	0.00	0.032973210	0.063206490
3	128	Tanhshrink	LogCosh	0.00	9.999999999	9.999999999
5	256	CELU	MAE	0.01	0.045101840	0.079573950
5	256	Leaky ReLU	MAE	0.01	0.052348200	0.050300210
3	128	Sigmoid	MSE+MAE	0.00	0.021113300	0.039422370
4	128	Tanh	MSE+MAE	0.00	0.009787550	0.054194300

Continued on next page

Table S4 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
5	128	ReLU	MSE	0.00	0.032394820	0.060825720
5	32	ReLU	MAE	0.00	0.035884530	0.047156700
4	256	Sigmoid	LogCosh	0.00	0.067027860	0.071537770
4	128	Sigmoid	LogCosh	0.01	0.656490910	0.713837010
4	128	ReLU	MAE	0.00	0.017021570	0.083774410
4	256	ReLU	MAE	0.00	0.029627020	0.048390410
5	128	Tanhshrink	LogCosh	0.01	9.999999999	9.999999999
5	128	RReLU	MSE+MAE	0.00	0.036556520	0.054125190
4	256	ReLU	MSE	0.00	0.001221960	0.065955870
5	128	Leaky ReLU	MSE	0.01	0.071020910	0.118922080
5	64	Tanh	MSE+MAE	0.00	0.021320290	0.038056540
5	128	Leaky ReLU	MSE+MAE	0.00	0.001953160	0.044955800
5	128	Tanh	LogCosh	0.05	0.534014200	0.515616370
5	256	Sigmoid	MAE	0.00	2.742521480	2.838006540
5	128	SELU	LogCosh	0.00	0.032226770	0.053437190
4	256	CELU	MAE	0.00	0.034502390	0.063281080
5	256	RReLU	LogCosh	0.00	0.121556160	0.131477550
3	128	RReLU	LogCosh	0.00	0.505236540	0.552226020
3	128	ReLU	MAE	0.00	0.024244380	0.077055360
4	32	Sigmoid	MAE	0.00	0.056026760	0.087484300
4	256	ReLU	LogCosh	0.01	0.171202140	0.181599520
5	128	ReLU	MAE	0.05	0.126414900	0.149547920
5	256	Tanh	MSE	0.00	0.038525670	0.044253440
5	64	ReLU	MAE	0.05	0.178048580	0.184771020
5	32	Tanh	LogCosh	0.05	0.170648770	0.186544950
5	128	ReLU	MSE+MAE	0.00	0.019375510	0.067992910
5	128	RReLU	LogCosh	0.01	0.275863940	0.278381930
4	128	Sigmoid	MAE	0.00	0.039371860	0.035245950
5	64	ReLU	LogCosh	0.00	0.007102880	0.053127150
4	256	ReLU	MSE+MAE	0.00	0.027942030	0.056231630
5	128	Tanh	MSE	0.00	0.012026620	0.037387790
5	128	RReLU	MAE	0.05	0.112849740	0.134798670
5	256	RReLU	MSE	0.00	0.045277070	0.057576930
5	128	CELU	MSE	0.00	0.003617820	0.045101560
4	128	Tanhshrink	LogCosh	0.00	9.999999999	9.999999999
3	64	ReLU	MAE	0.00	0.023432670	0.082240470
5	32	Sigmoid	LogCosh	0.05	0.153291340	0.168882560
5	32	Tanhshrink	MSE+MAE	0.00	2.761885030	2.599543900
5	256	SELU	LogCosh	0.01	0.550440350	0.631587340
5	128	Tanh	MSE+MAE	0.01	0.073421480	0.113590680

Continued on next page

Table S4 – Continued from previous page

Layers	Neurons	Activation Func.	Loss Func.	Dropout	Performance Training	Performance Test
5	256	CELU	MSE	0.00	0.030675530	0.060089870
5	32	Tanhshrink	MAE	0.05	4.412677470	4.287058430
5	256	SELU	MSE+MAE	0.05	0.075563550	0.080276350
5	32	Sigmoid	MSE+MAE	0.00	2.747330410	2.684238140
5	64	CELU	MSE	0.00	0.036305770	0.046708640
5	256	Tanhshrink	MSE+MAE	0.00	9.999999999	9.999999999
3	128	Sigmoid	LogCosh	0.05	0.047734720	0.120873100
5	256	Tanhshrink	MAE	0.05	2.745595200	2.827288310
5	256	SELU	LogCosh	0.05	0.515861210	0.543625420
5	32	Tanh	LogCosh	0.00	0.012517780	0.033415450
5	256	Leaky ReLU	MSE+MAE	0.00	0.018022070	0.044067330
5	128	Tanhshrink	MSE+MAE	0.05	2.757121930	2.627898940
5	256	Tanh	LogCosh	0.01	0.097008690	0.111512660
3	32	Sigmoid	LogCosh	0.00	0.046516150	0.047769490
3	256	ReLU	MSE+MAE	0.00	0.015989940	0.048940320
5	256	Leaky ReLU	MSE+MAE	0.05	0.106226250	0.112153160
5	128	Sigmoid	MSE	0.01	2.777008020	2.943130360
5	128	RReLU	LogCosh	0.05	0.229303390	0.215375560
4	64	ReLU	MAE	0.00	0.031699560	0.066728010
5	32	Leaky ReLU	MAE	0.00	0.043359920	0.063762120
3	256	Tanh	MSE	0.00	0.015555320	0.034141440
5	128	Tanh	MAE	0.00	2.755675840	2.755261280
5	256	Leaky ReLU	LogCosh	0.00	0.019402080	0.050034430
3	128	Sigmoid	MSE	0.00	0.000323340	0.062589260
3	256	SELU	MAE	0.00	0.035897180	0.039190850
5	128	Leaky ReLU	MAE	0.01	0.057982860	0.100748650
3	256	Tanh	LogCosh	0.05	0.084280990	0.100934190
5	128	Sigmoid	MSE+MAE	0.01	1.030789270	0.941872100
3	64	ReLU	MSE	0.00	0.031477630	0.059369500
5	256	Sigmoid	LogCosh	0.05	9.999999999	9.999999999
5	256	Tanh	MAE	0.00	0.037948170	0.043290640
5	256	Leaky ReLU	MAE	0.05	0.109857560	0.119878100
5	64	Sigmoid	MSE+MAE	0.00	0.038005490	0.040226030
3	64	CELU	MAE	0.00	0.041930630	0.049845510
5	32	Sigmoid	LogCosh	0.01	0.724041740	0.745168930
5	128	SELU	LogCosh	0.05	2.720189140	2.932994390
3	256	Leaky ReLU	MAE	0.00	0.029513830	0.047320900
5	128	Tanh	MSE+MAE	0.05	1.533308200	1.539373330
3	256	ReLU	MSE	0.00	0.000653240	0.055673670
5	32	Tanhshrink	MAE	0.00	2.760321540	2.773767940
3	256	SELU	LogCosh	0.00	9.999999999	9.999999999

