Supporting information

Supporting figures

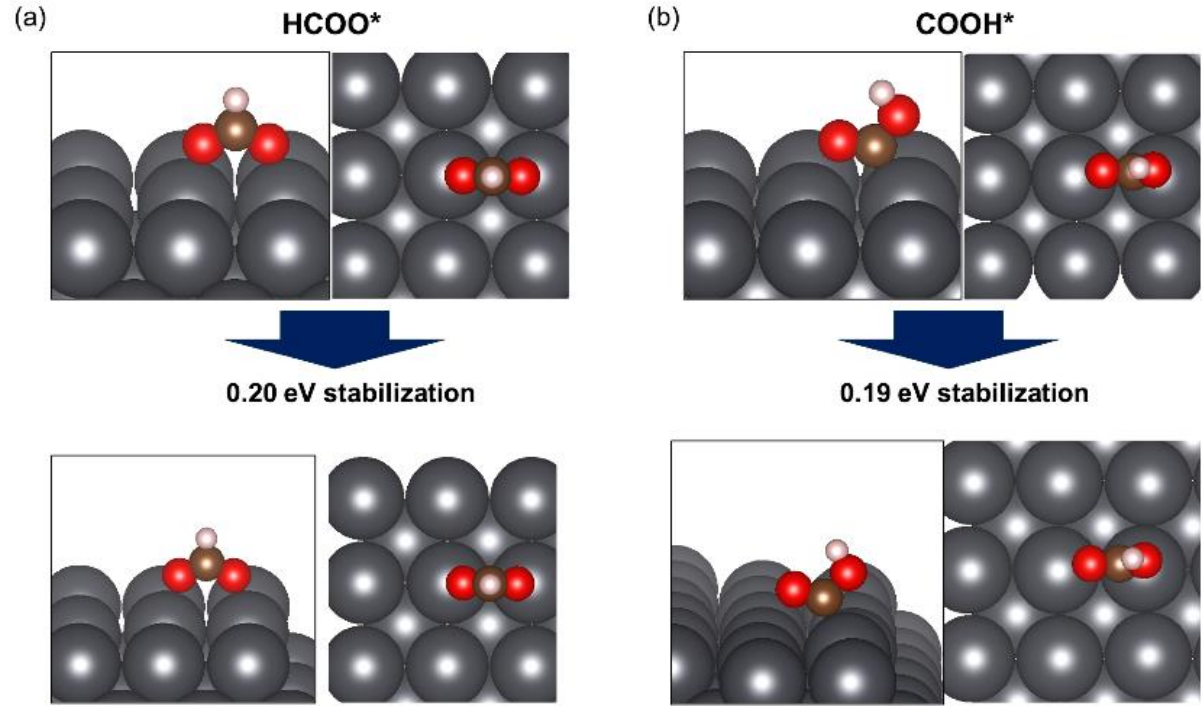

Figure S1. *Illustration of configurational change from vacuum to implicit solvation for (a) HCOO* adsorbate and (b) COOH* adsorbate. As discussed in the main text, both configuration in implicit solvation do not change significantly compared to the vacuum case configurations.*

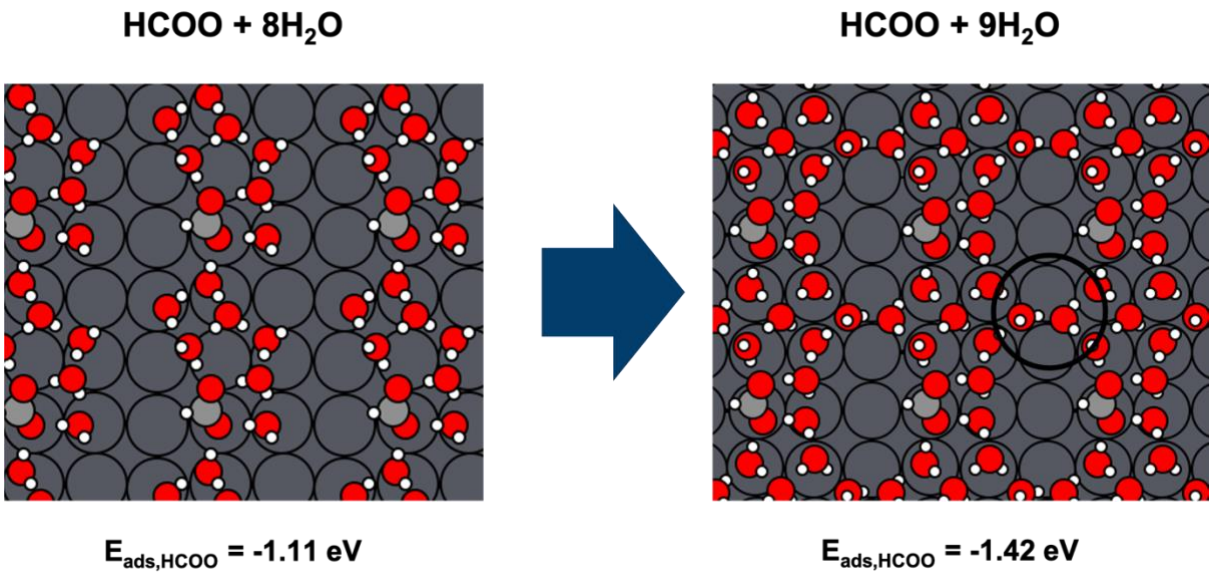

Figure S2. *HCOO adsorbate in the presence of eight and nine explicit water molecules. Adsorption energy ($E_{ads,HCOO}$) increases from eight to nine water molecules due to additional H-bonding caused by periodic boundary conditions.*

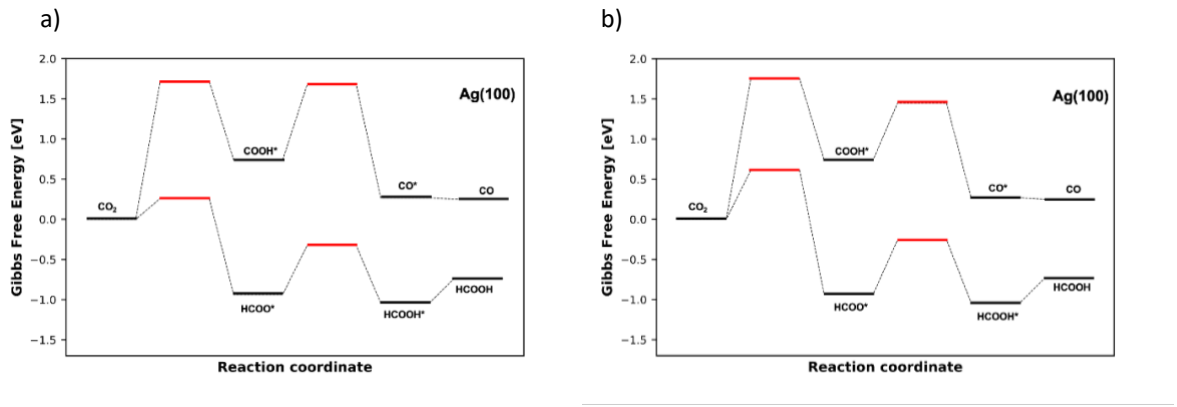

Figure S3.1 *Free energy diagram for CO_2 reduction towards CO and HCOOH via HCOO* and COOH* reaction intermediate under implicit solvation environment on Ag(100) surface using a) single point (SP) calculation method and b) nudged elastic band (NEB) method to calculate the activation energies (indicate in red).*

As shown in Figure S3.1, we have compared two different implicit solvation methods to calculate the reaction pathway on the Ag(100) surface. The implicit nudged elastic band (NEB) method performs a series of energy minimizations along the reaction pathway under implicit solvation, while the implicit single point (SP) method uses the same reaction pathway as the vacuum case. During the implicit SP method, implicit single point calculations are applied to the vacuum reaction pathway to calculate the activation barriers under implicit solvation. The SP method is computationally more efficient since only single point calculations are performed. Our results in Figure S3.1 show similar reaction energy trends among these methods. Regardless of the implicit solvation method used, the HCOO* pathway is favored over the COOH* pathway, leading to HCOOH formation on Ag(100). In both cases, microkinetic modeling results in selectivities of $s_{CO} \approx 0$ and $s_{HCOOH} \approx 1$ on the Ag(100) surface, confirming the previous findings observed in the vacuum case.

During implicit NEB method calculations, we encountered some convergence difficulties. To bypass this, we increased the α parameter from 1.18 up to 1.9. The α parameter in the Environ package corresponds to the homogeneous scaling factor of the solvent radii. Increasing the α parameter creates a bigger distance between solute cavity and implicit solvation. For implicit SP calculations, we experienced no convergence issues even for α values of 1.18.

In order to validate the findings obtained from our implicit solvation calculations on the Ag(100) surface, we have performed similar implicit NEB calculations using the VASPsol package [1,2]. As shown in Figure S3.2, the HCOO* activation energy is significantly lower than the COOH* activation energy, favoring the HCOO* pathway over the COOH* pathway. Also here, HCOOH formation is favored over CO, supporting the aforementioned observations. Quantitative differences between VASPsol and Environ arise due to variations in the dielectric functions utilized to describe the implicit solvation environment. Despite these differences, here the microkinetic modeling also demonstrates selectivities of $s_{CO} \approx 0$ and $s_{HCOOH} \approx 1$ on the Ag(100) surface, indicating that CO cannot be predicted as the primary product on the Ag(100) surface, regardless of the implicit solvation method used.

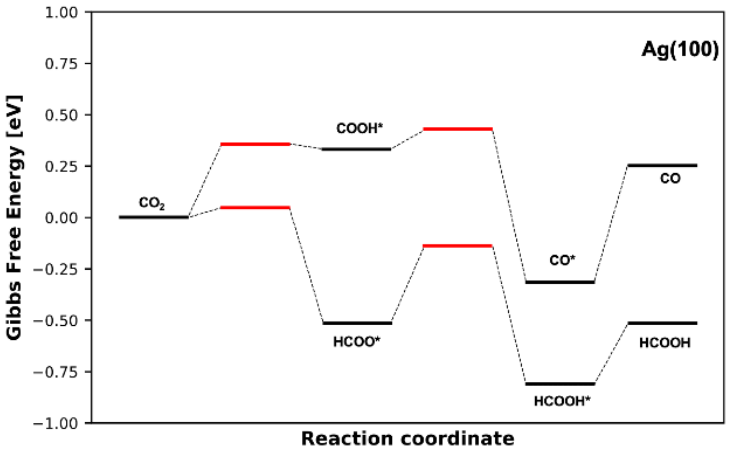

Figure S3.2 *Free energy diagram for CO_2 reduction towards CO and HCOOH via HCOO* and COOH* reaction intermediate under implicit solvation environment on Ag(100) surface using VASPsol.*

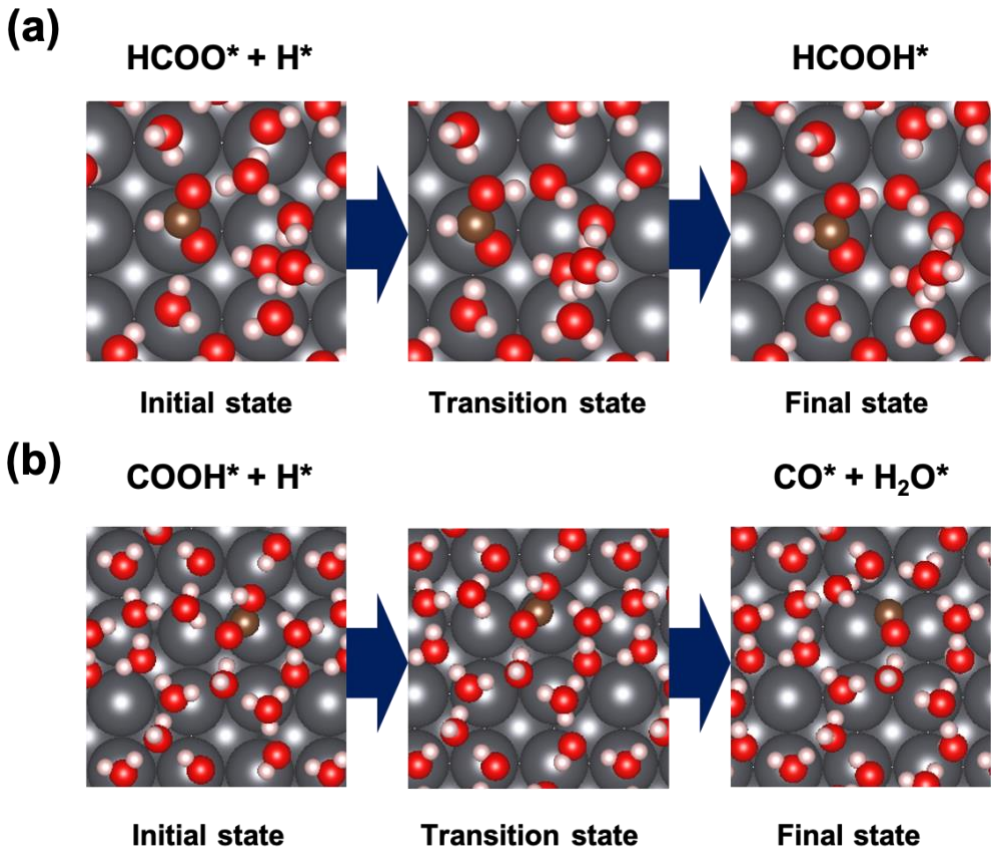

Figure S4. *Illustration of H_3O^+-mechanism from (a) HCOO* to HCOOH* and (b) COOH* to CO*+ H_2O* on Pb(100) surface. H* indicates the presence of H_3O^+, which supplies a proton to the HCOO*/COOH* reaction intermediate.*

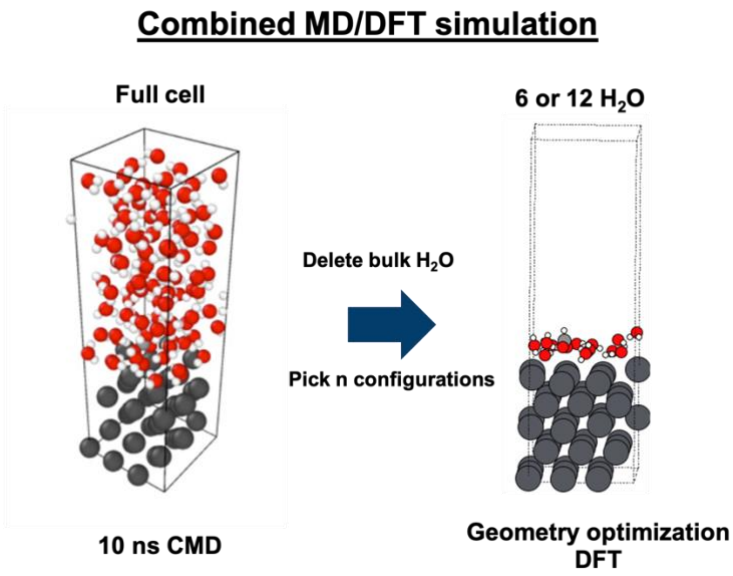

Figure S5. *Workflow of combined MD/DFT simulation. Initially, we run a 10ns CMD simulation of a simulation cell filled completely with explicit water molecules, where n different, independent configurations are selected from the CMD simulation. After that, we removed all bulk water molecules from the system except the remaining 6 or 12 explicit water molecules closest to the Pb surface. Lastly, we ran DFT geometry optimizations from the given configurations.*

Pb(100)	$E_{ads,H2O}$**[eV]**	
Variables	6 H_2O	12 H_2O
Mean	-0.32	-0.42
Min	-0.35	-0.43
Max	-0.27	-0.40
SD	0.02	0.01

Figure S6. *Statistical mean, minimum (Min), maximum (Max) and standard deviation (SD) of H_2O adsorption energies, $E_{ads,H2O}$, on Pb(100) surface in the presence of 6 and 12 explicit water molecules from the combined MD/DFT method. The sample size is n = 19. As already observed in the main text, the uncertainty ranges for water configurations are much lower than for HCOO and COOH adsorbates, with adsorption energies varying up to only 0.1 eV.*

Pb(100) Variables	$E_{ads,HCOO}$[eV] n=19	n=38
Mean	-1.01	-1.03
Min	-1.28	-1.37
Max	-0.48	-0.48
SD	0.21	0.22

Figure S7. *Statistical mean, minimum (Min), maximum (Max) and standard deviation (SD) of HCOO adsorption energy, $E_{ads,HCOO}$, on Pb(100) surface in the presence of 12 explicit water molecules from the combined MD/DFT method using a sample size of n = 19 and n = 38 configurations.*

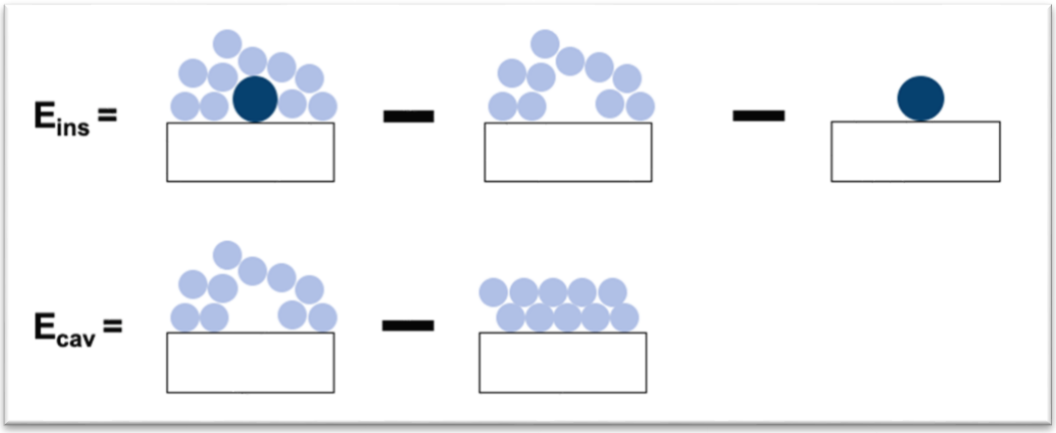

Figure S8. *Illustration of adsorbate insertion energy E_{ins} and cavitation energy E_{cav}.*

The mathematical definition of the adsorbate insertion energy, E_{ins}, is

$$E_{ins} = E_{adsorbate,nH20} - E_{nH2O} - E_{adsorbate}$$

where $E_{adsorbate,nH20}$, E_{nH2O} and $E_{adsorbate}$ represent the energy of the adsorbate in presence of n explicit water molecules, the energy of the same water configuration without the adsorbate and the energy of the same adsorbate configuration without the explicit water molecules.

The mathematical definition of the cavitation energy, E_{cav}, is

$$E_{cav} = E_{nH2O} - E_{nH2O,optimized}$$

where E_{nH2O} and $E_{nH2O,optimized}$ represent the energy of the same unoptimized water configuration when the adsorbate is removed and the energy of the optimized water configuration.

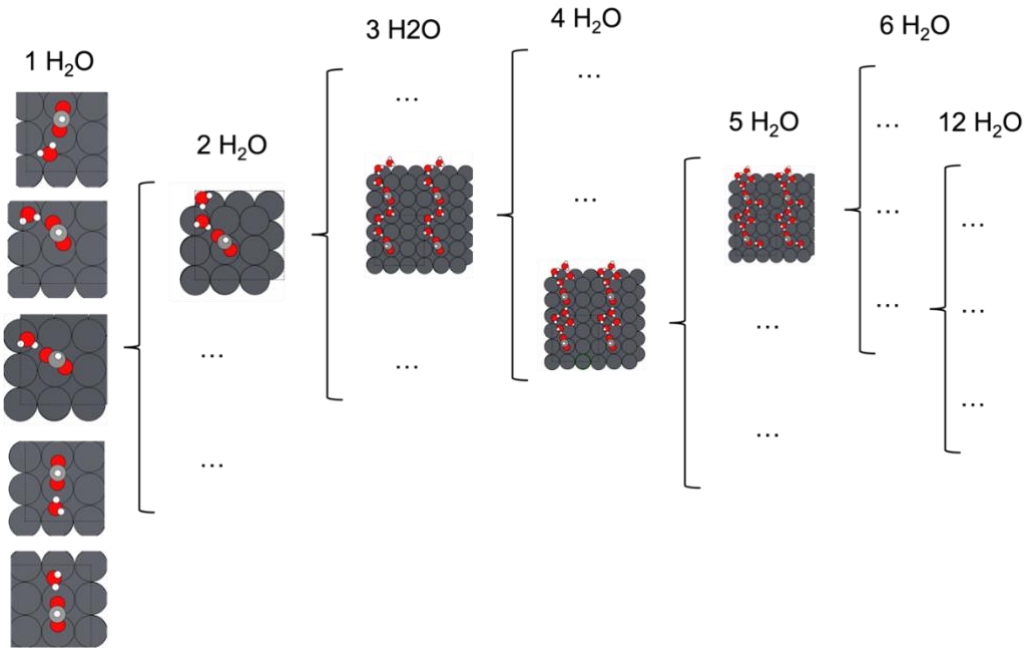

Figure S9. *Initialization of explicit water structures for 1-12 water molecules. Starting with one explicit water molecule, the most energetically stable configuration is taken to use a basis for the initialization of two explicit water configuration. This procedure is repeated up until 12 explicit water molecules.*

(a)

Molecule	ZPE	TS
H_2O	0.56	0.67
CO_2	0.31	0.66
H_2	0.27	0.43
CO	0.13	0.67
HCOOH	0.89	1.05

(b)

Ag(100) surface	ZPE	TS
COOH*	0.58	0.29
HCOO*	0.60	0.24
CO*	0.17	0.21
HCOOH*	0.90	0.31

(c)

Pb(100) surface	ZPE	TS
COOH*	0.58	0.27
HCOO*	0.61	0.17
CO*	0.16	0.21
HCOOH*	0.91	0.29

Figure S10. *Zero-point energy (ZPE) and entropy (TS) correction terms for (a) different gas phase molecules and adsorbates at (b) Ag(100) surface and (c) Pb(100) surface given in eV. Gas phase correction values are taken from ref[3].*

Microkinetic modeling

When taking into account explicit solvation effects, we examine the following mechanism for the microkinetic model:

$$\mathrm{CO_2} + * \rightleftharpoons \mathrm{CO_2}* \quad \text{(Step 5)}$$

$$\mathrm{CO_2}* + \mathrm{H^+} + \mathrm{e^-} + * \rightleftharpoons \mathrm{HCOO}* \quad \text{(Step 6)}$$

$$\mathrm{HCOO}* + \mathrm{H^+} + \mathrm{e^-} \rightarrow \mathrm{HCOOH} + 2* \quad \text{(Step 7)}$$

$$\mathrm{CO_2}* + \mathrm{H^+} + \mathrm{e^-} \rightleftharpoons \mathrm{COOH}* \quad \text{(Step 8)}$$

$$\mathrm{COOH}* + \mathrm{H^+} + \mathrm{e^-} \rightarrow \mathrm{CO} + \mathrm{H_2O} + * \quad \text{(Step 9)}$$

where * indicates a free adsorption site.
In the same logic as in the vacuum case, we solve the rate equations at steady state

$$\frac{d\theta_{\mathrm{CO_2}*}}{dt} = v_5 - v_6 - v_8 = 0 \quad (10)$$

$$\frac{d\theta_{\mathrm{HCOO}*}}{dt} = v_6 - v_7 = 0 \quad (11)$$

$$\frac{d\theta_{\mathrm{COOH}*}}{dt} = v_8 - v_9 = 0 \quad (12)$$

For v_i, we have the following relations

$$v_5 = k_5 c_{\mathrm{CO_2}} \theta_0 - k_{-5} \theta_{\mathrm{CO_2}*} \quad (13)$$

$$v_6 = k_6 \theta_{\mathrm{CO_2}*} c_{\mathrm{H^+}} \theta_0 - k_{-6} \theta_{\mathrm{HCOO}*} \quad (14)$$

$$v_7 = k_7 \theta_{\mathrm{HCOO}*} c_{\mathrm{H^+}} \quad (15)$$

$$v_8 = k_8 \theta_{\mathrm{CO_2}*} c_{\mathrm{H^+}} - k_{-8} \theta_{\mathrm{COOH}*} \quad (16)$$

$$v_9 = k_9 \theta_{\mathrm{COOH}*} c_{\mathrm{H^+}} \quad (17)$$

with $c_{\mathrm{CO_2}} = 0.034$ M and $c_{\mathrm{H^+}} = 1$ M, corresponding to $p_{\mathrm{CO_2}} = 1$ atm and pH = 0. The selectivities of CO and HCOOH are given by

$$s_{CO} = \frac{v_9}{v_7 + v_9} \quad (18)$$

$$s_{HCOOH} = \frac{v_7}{v_7 + v_9} \quad (19)$$

Given the activation barriers in Figure 4, we obtain $s_{CO} \approx 1$ and $s_{HCOOH} \approx 0$ for Ag(100), and $s_{CO} \approx 0$ and $s_{HCOOH} \approx 1$ for Pb(100).

XYZ-coordinate files

Figure 1

HCOO* in vacuum:
49
Lattice="10.6702413281 0.0 0.0 0.0 10.6702413281 0.0 0.0 0.0 35.21"
Properties=species:S:1:pos:R:3
Pb 7.11352979 3.55671154 11.3175503
Pb 3.55671154 0.0 11.3175503
Pb 0.0 7.11352979 11.3175503
Pb 0.0 0.0 11.3175503
Pb 7.11352979 0.0 11.3175503
Pb 3.55671154 3.55671154 11.3175503
Pb 0.0 3.55671154 11.3175503
Pb 7.11352979 7.11352979 11.3175503
Pb 3.55671154 7.11352979 11.3175503
Pb 8.89183221 8.89183221 13.8326006
Pb 5.33512066 5.33512066 13.8326006
Pb 5.33512066 1.77840912 13.8326006
Pb 8.89183221 1.77840912 13.8326006
Pb 1.77840912 8.89183221 13.8326006
Pb 1.77840912 5.33512066 13.8326006
Pb 8.89183221 5.33512066 13.8326006
Pb 1.77840912 1.77840912 13.8326006
Pb 5.33512066 8.89183221 13.8326006
Pb 0.02049504 5.47e-04 16.4421122
Pb 7.11170126 7.1002806 16.39897244
Pb 3.5561695 3.55773414 16.41109523
Pb 0.01108162 7.09981669 16.39174612
Pb 7.09969366 -0.00278905 16.44514749
Pb 3.56154235 7.11380651 16.41322364
Pb 0.00359485 3.57058484 16.39658071
Pb 3.55856805 1.0103e-04 16.35374069
Pb 7.10812463 3.57066739 16.39557252
Pb 8.89702882 8.88120232 18.97390329
Pb 8.89230091 1.77820059 18.97843677
Pb 8.88834952 5.32956545 18.97853931
Pb 5.33824176 5.33290045 18.96078671
Pb 5.34414932 8.8996784 18.94073488
Pb 5.33715843 1.77488042 18.94212574
Pb 1.7808276 8.89866688 18.93826382
Pb 1.7666507 5.33595021 18.95469923
Pb 1.77602879 1.77192137 18.93827619
Pb 7.09264289 7.12083766 21.30566385
Pb 7.08451679 3.54042703 21.30588059
Pb 0.01896203 3.54096665 21.30474312

Pb 7.12669817 -0.00733675 21.32100063
Pb 3.56354097 7.07406886 21.54914312
Pb 0.02813282 7.12156598 21.3004494
Pb 3.54926584 3.61971966 21.54881498
Pb 0.0034642 -0.00268814 21.31852179
Pb 3.56443201 0.00773985 21.26298028
C 3.60004231 5.35987845 24.50125646
O 3.56966922 4.21780501 23.95312436
H 3.62988193 5.35710883 25.61555023
O 3.60137015 6.50543675 23.95767341

COOH* in vacuum:
49
Lattice="10.6702413858 0.0 0.0 0.0 10.6702413858 0.0 0.0 0.0 35.2100039727"
Properties=species:S:1:pos:R:3
Pb 7.11352979 3.55671154 11.3175503
Pb 3.55671154 0.0 11.3175503
Pb 0.0 7.11352979 11.3175503
Pb 0.0 0.0 11.3175503
Pb 7.11352979 0.0 11.3175503
Pb 3.55671154 3.55671154 11.3175503
Pb 0.0 3.55671154 11.3175503
Pb 7.11352979 7.11352979 11.3175503
Pb 3.55671154 7.11352979 11.3175503
Pb 8.89183221 8.89183221 13.8326006
Pb 5.33512066 5.33512066 13.8326006
Pb 5.33512066 1.77840912 13.8326006
Pb 8.89183221 1.77840912 13.8326006
Pb 1.77840912 8.89183221 13.8326006
Pb 1.77840912 5.33512066 13.8326006
Pb 8.89183221 5.33512066 13.8326006
Pb 1.77840912 1.77840912 13.8326006
Pb 5.33512066 8.89183221 13.8326006
Pb 10.64233525 0.02214425 16.44817765
Pb 7.08925552 7.11977935 16.38399013
Pb 3.55766484 3.56694973 16.39499709
Pb 10.64063756 7.10727038 16.45276995
Pb 7.08936395 0.00705497 16.380847
Pb 3.56144503 7.11585548 16.42213292
Pb 10.67219359 3.56849775 16.35335448
Pb 3.56403536 0.01619265 16.42409841
Pb 7.11030564 3.5655985 16.46747337
Pb 8.88546763 8.89556898 18.99044319
Pb 8.9233673 1.76582534 18.91439635
Pb 8.92180021 5.35880007 18.92742733
Pb 5.3197654 5.33674061 19.02471277
Pb 5.34497903 8.90231959 18.9944096

Pb 5.31855428 1.79846159 18.99709854
Pb 1.79247854 8.89925984 18.98945707
Pb 1.7834574 5.34696937 18.95862709
Pb 1.78288402 1.78058575 18.95482933
Pb 7.12879626 7.08783045 21.32171859
Pb 6.99970139 3.60677969 21.63935874
Pb -0.05373548 3.56265159 21.27198299
Pb 7.12079971 0.09498615 21.30974292
Pb 3.53778478 7.13452416 21.34390403
Pb 0.01467452 7.12876335 21.33478083
Pb 3.44008343 3.57222744 21.44955222
Pb 0.01020495 10.66936721 21.32639111
Pb 3.54246289 0.02553537 21.33961473
C 5.84299877 3.81319668 23.8252787
O 6.68865031 3.92233805 24.88857552
O 4.62383082 3.82340977 24.01058659
H 6.13413408 3.99065109 25.70437567

HCOO* with 12 explicit water molecules:
85
Lattice="10.6702413858 0.0 0.0 0.0 10.6702413858 0.0 0.0 0.0 35.2100039727"
Properties=species:S:1:pos:R:3
Pb 7.11352979 3.55671154 11.3175503
Pb 3.55671154 0.0 11.3175503
Pb 0.0 7.11352979 11.3175503
Pb 0.0 0.0 11.3175503
Pb 7.11352979 0.0 11.3175503
Pb 3.55671154 3.55671154 11.3175503
Pb 0.0 3.55671154 11.3175503
Pb 7.11352979 7.11352979 11.3175503
Pb 3.55671154 7.11352979 11.3175503
Pb 8.89183221 8.89183221 13.8326006
Pb 5.33512066 5.33512066 13.8326006
Pb 5.33512066 1.77840912 13.8326006
Pb 8.89183221 1.77840912 13.8326006
Pb 1.77840912 8.89183221 13.8326006
Pb 1.77840912 5.33512066 13.8326006
Pb 8.89183221 5.33512066 13.8326006
Pb 1.77840912 1.77840912 13.8326006
Pb 5.33512066 8.89183221 13.8326006
Pb 8.7234e-04 -0.00221799 16.39721847
Pb 7.11533908 7.1171553 16.42529341
Pb 3.57068739 3.5651257 16.39197342
Pb 0.00948178 7.11612909 16.40702274
Pb 7.12141859 -0.00108643 16.36493448
Pb 3.56775666 7.1108381 16.37493864
Pb 0.00446613 3.5620321 16.42710542

Pb 3.57030323 -0.0039016 16.43035104
Pb 7.11638091 3.55544955 16.39620343
Pb 8.90032077 8.88953854 18.94494518
Pb 8.89717338 1.77406794 18.96271742
Pb 8.90118925 5.32425468 18.93905817
Pb 5.35082268 5.32665177 18.93330103
Pb 5.34742526 8.88540249 18.91445848
Pb 5.35868048 1.78274293 18.93702631
Pb 1.78604961 8.89011664 18.95060423
Pb 1.79639403 5.33932782 18.96559664
Pb 1.78400727 1.78568814 18.9405481
Pb 7.14091564 7.11639969 21.46510932
Pb 7.14819148 3.54780792 21.3758915
Pb 0.00929436 3.56030802 21.30587522
Pb 7.09358722 -0.02177498 21.26293663
Pb 3.60832691 7.15183639 21.2738277
Pb -0.00471681 7.10914368 21.29789865
Pb 3.59305099 3.5405762 21.28366372
Pb 0.03109077 0.00697472 21.29080419
Pb 3.57398347 0.02828583 21.46712927
C 3.68891533 3.66480098 25.17540623
O 4.39454904 2.69164276 24.7722291
H 2.60778765 3.45791818 25.36055874
O 4.09108172 4.84816279 25.37924874
O 2.86570044 7.14037826 25.9667263
H 2.69720336 7.13471825 26.92358274
H 3.2637761 6.23558183 25.75720532
O 1.32625425 9.06125032 24.48400064
H 1.83231901 8.35883741 24.95623706
H 1.94101799 9.83346522 24.45554638
O 3.4704989 10.89795495 24.16855907
H 3.73690439 11.82716114 24.44857188
H 4.16100783 10.28596881 24.55611463
O 5.20038847 9.13886427 25.31531228
H 4.60281147 8.4691984 25.71258853
H 5.86578523 8.61658097 24.77862706
O 6.58189909 5.85651874 25.76774182
H 5.73203036 5.3699918 25.59112992
H 7.27518301 5.17870304 25.97799479
O 7.12511919 2.42405396 24.31559165
H 6.16578688 2.59953669 24.52456231
H 7.31848895 1.55018695 24.73424835
O 7.15512923 7.69470044 24.06822305
H 6.98108951 6.89412973 24.69855988
H 8.02106628 8.08743786 24.37131995
O 9.40009325 8.71102496 25.3049581
H 9.60391953 7.86432818 25.79225943

H 10.29185349 8.9847501 24.95333881
O 7.60520049 10.72808239 25.92727638
H 8.28774434 10.01831936 25.77187383
H 6.74846308 10.24971019 25.99196752
O 8.62930098 4.03045054 26.01512126
H 8.21643251 3.5094388 25.2750727
H 8.62510941 3.37731925 26.76738968
O -0.44264709 6.28261437 26.32265543
H 0.45099641 6.14506786 25.96447005
H -0.94698696 5.44494328 26.14715441
O 8.36441784 1.95331736 27.79047879
H 9.06061749 1.60315342 28.36726731
H 8.0912445 1.19829164 27.20428

COOH* with 12 explicit water molecules:
85
Lattice="10.6702413281 0.0 0.0 0.0 10.6702413281 0.0 0.0 0.0 35.21"
Properties=species:S:1:pos:R:3
Pb 7.11352979 3.55671154 11.3175503
Pb 3.55671154 0.0 11.3175503
Pb 0.0 7.11352979 11.3175503
Pb 0.0 0.0 11.3175503
Pb 7.11352979 0.0 11.3175503
Pb 3.55671154 3.55671154 11.3175503
Pb 0.0 3.55671154 11.3175503
Pb 7.11352979 7.11352979 11.3175503
Pb 3.55671154 7.11352979 11.3175503
Pb 8.89183221 8.89183221 13.8326006
Pb 5.33512066 5.33512066 13.8326006
Pb 5.33512066 1.77840912 13.8326006
Pb 8.89183221 1.77840912 13.8326006
Pb 1.77840912 8.89183221 13.8326006
Pb 1.77840912 5.33512066 13.8326006
Pb 8.89183221 5.33512066 13.8326006
Pb 1.77840912 1.77840912 13.8326006
Pb 5.33512066 8.89183221 13.8326006
Pb 10.64221305 0.02243859 16.42854634
Pb 7.08294225 7.11297954 16.35606239
Pb 3.54133824 3.58387109 16.38680199
Pb 10.63117375 7.11569839 16.49951785
Pb 7.10928655 0.01534394 16.38504985
Pb 3.55675678 7.10976935 16.44450558
Pb 10.64800897 3.58204512 16.38734587
Pb 3.56084596 0.03080295 16.51323309
Pb 7.09595401 3.56785211 16.47072567
Pb 8.83944623 8.89881852 18.97368067

Pb 8.85287395 1.80917129 18.94756143
Pb 8.83173194 5.3655682 18.91160756
Pb 5.31057541 5.35487041 18.99822838
Pb 5.35380735 8.90132322 18.99338708
Pb 5.32514716 1.81357785 18.96839327
Pb 1.77917094 8.88937494 18.97325485
Pb 1.75833302 5.34022392 18.98585928
Pb 1.74803192 1.78042823 19.02615296
Pb 7.13560592 7.08771718 21.42050044
Pb 6.86344057 3.71157761 21.98804766
Pb 10.45979635 3.64361789 21.30858922
Pb 7.06731878 0.2086418 21.3622377
Pb 3.52140111 7.17395589 21.33616959
Pb 10.66033659 7.11107005 21.49021882
Pb 3.55981729 3.55584278 21.32139539
Pb 10.5956447 10.58344224 21.27102754
Pb 3.58238075 10.63684284 21.42701753
C 6.07190775 4.00994035 24.44719058
O 6.77072095 4.93276784 25.25361775
O 5.08093206 3.49741257 24.99141907
O 4.93283639 0.87670011 25.79392711
H 6.29114959 4.9758309 26.1208985
H 5.0333781 1.82313114 25.50448588
H 4.71375694 0.91311269 26.74167143
O 7.20631795 9.77981677 25.71719466
H 6.40919417 10.35472968 25.66771892
H 7.9742571 10.39501521 25.64241259
O 9.3726244 0.88680504 25.11830553
H 9.21405506 1.81271128 25.5170437
H 9.03632561 0.93105241 24.1992053
O 7.75186929 7.53463856 24.3764093
H 7.32221998 6.7531255 24.78155932
H 7.46112835 8.35325941 24.88353583
O 10.40991951 7.11679435 24.23051112
H 9.42347833 7.27187959 24.35157417
H 0.18287108 7.94297328 24.57154057
O 9.15505875 3.31780991 26.11196319
H 8.40712526 3.86140289 25.79249432
H 9.9756138 3.86435073 25.94009957
O 0.88709691 9.40609215 25.24553117
H 1.57309943 9.99602074 24.80122187
H 0.16575465 10.01710874 25.50291458
O 2.75861376 0.32786326 24.19477015
H 3.52789032 0.46137683 24.80939224
H 2.27351031 1.20644391 24.15306957
O 0.6544141 4.7234484 25.31768066
H 0.3528939 5.58073676 24.90909511

H 1.51975432 4.92035674 25.79793031
O 3.0317932 5.22394356 26.41809134
H 3.20112076 6.17990153 26.20176783
H 3.69638639 4.69308924 25.93136064
O 3.25747521 7.9086941 25.84435133
H 3.58253497 8.11727066 24.94998428
H 2.38015338 8.35510093 25.89909171
O 1.06499283 2.38441028 24.0521578
H 0.31096615 1.88562602 24.43769368
H 0.99505486 3.30114584 24.45387723

Figure 6

Configuration 1:
85
Lattice="10.6877079379 0.0 0.0 0.0 10.6790508945 0.0 0.0 0.0 35.2100018514"
Properties=species:S:1:pos:R:3
Pb 3.55670995 0.0 0.31754997
Pb 0.0 0.0 0.31754997
Pb 3.55670995 3.55670995 0.31754997
Pb 0.0 3.55670995 0.31754997
Pb 1.77841002 5.33511997 2.83259957
Pb 1.77841002 1.77841002 2.83259957
Pb 1.75276914 1.71726457 7.93261883
Pb 1.77360803 5.25212565 7.96121486
H -0.45834342 2.120313 15.51366123
H 0.28784028 3.50816211 15.64260095
O 0.27708631 2.58378653 15.98568065
Pb -0.0381113 -0.1341457 10.45151707
Pb -0.04796964 3.45337585 10.38209507
Pb 3.53027712 3.37796766 10.50670092
O 3.3373191 5.21961257 14.17125091
C 3.89187754 6.34364309 14.34567431
H 1.70068473 1.9566874 15.6329446
H 3.25898461 7.15053939 14.78378483
Pb 0.0 7.11352999 0.31754997
Pb 3.55670995 7.11352999 0.31754997
Pb 1.77841002 8.89182993 2.83259957
Pb 1.76180239 8.81817452 7.95642463
O 0.65264168 5.07127253 14.61876234
H 0.25761544 5.97277214 14.65559005
O 2.28725607 9.76737872 14.27221128
H 1.64104091 5.16774726 14.45860063
H 3.18053149 9.55344821 13.91147762
H 3.15324043 12.2808241 16.18252792
H 2.41343408 10.63163702 14.74701484
O 5.09051895 6.65885993 14.06144754

O 2.60716589 12.23739994 15.38115717
Pb 7.11352999 3.55670995 0.31754997
Pb 7.11352999 0.0 0.31754997
Pb 5.33511997 5.33511997 2.83259957
Pb 5.33511997 1.77841002 2.83259957
Pb 5.30721009 1.68740419 7.95416952
Pb 5.31930965 5.25569962 7.95464192
Pb 3.55186735 3.50239609 5.43986913
Pb 3.54311947 -0.06196199 5.39078904
Pb 7.01859856 3.42063406 10.25572575
H 4.07476026 3.72672253 13.65790106
O 4.19827276 2.77495863 13.37576481
Pb 3.49090894 -0.08620598 10.25877281
H 3.56697015 2.30313052 13.97738872
H 5.72983413 1.71631016 13.85568137
Pb 7.11352999 7.11352999 0.31754997
Pb 5.33511997 8.89182993 2.83259957
Pb 5.33152997 8.82391382 7.9592013
Pb 7.1104872 7.06608619 5.44867794
Pb 3.53696441 7.06291194 5.40885981
H 5.1439265 9.24738218 12.58952251
O 5.01128777 9.25993276 13.5579913
H 5.13671764 8.29222173 13.83877449
H 6.71883294 6.03931167 13.54288423
Pb 7.13003716 10.5554219 10.30614715
Pb 3.58215953 6.97755563 10.28285542
O 7.62562938 5.94801193 13.14537096
H 5.94487616 10.84190698 14.02136543
O 6.39925551 11.71212581 14.1010455
H 8.22154498 6.56229222 13.64706586
Pb 8.89182993 1.77841002 2.83259957
Pb 8.89182993 5.33511997 2.83259957
Pb 8.88772157 1.70196619 7.94774194
Pb 8.88114329 5.25672029 7.96798766
Pb 7.12041288 3.49880288 5.38181671
Pb 10.66835784 3.51243933 5.40381522
Pb 10.67483352 -0.05516033 5.42738696
O 9.53109274 3.84320679 13.00687537
H 9.22811545 2.18179939 13.67164439
H 8.76646098 4.4735336 13.06549744
O 9.12582661 1.33636107 14.1824698
H 8.13736966 1.20214591 14.23121537
H 10.2576645 4.28083957 13.54094441
Pb 8.89182993 8.89182993 2.83259957
Pb 8.89875449 8.82989787 7.94918905
Pb 10.67140277 7.047434 5.38823361
Pb 7.114074 10.62940542 5.40698947

Pb 10.68358141 7.02003927 10.26988803
Pb 7.14574595 6.98510008 10.4356982
O 9.6364917 7.43171268 14.46459109
H 9.38153002 7.68671391 15.36720329
H 9.92736943 8.29609388 14.02713679
H 10.01629116 10.54054247 13.64704449
H 11.4352415 9.76981124 13.62010933
O 10.47912129 9.72524778 13.30400647

Configuration 2:
85
Lattice="10.6877079379 0.0 0.0 0.0 10.6790508945 0.0 0.0 0.0 35.2100018514" Properties=species:S:1:pos:R:3
Pb 3.55671 0.0 0.31755
Pb 0.0 0.0 0.31755
Pb 3.55671 3.55671 0.31755
Pb 0.0 3.55671 0.31755
Pb 1.77841 5.33512 2.8326
Pb 1.77841 1.77841 2.8326
Pb 1.80548048 1.7014486 7.95086264
Pb 3.57032404 3.51464891 5.40338042
Pb 3.5776543 -0.05862959 5.43260957
Pb 0.00510618 3.5197779 5.38969579
Pb 3.61505263 3.46625034 10.31215205
Pb 3.5473137 -0.08414585 10.32868796
O 1.87060231 2.25877176 14.47338373
H 2.07359396 2.02730879 13.5491041
H 2.45089885 3.05079931 14.65387012
H -0.31266571 5.21472326 13.46610372
H 1.65845727 5.17264956 15.65146132
H 3.16770759 0.62189673 15.10356154
O 3.79787123 7.6178e-04 14.68151226
Pb 0.0 7.11353 0.31755
Pb 3.55671 7.11353 0.31755
Pb 1.77841 8.89183 2.8326
Pb 1.80674223 8.82153455 7.97142182
Pb 0.00258405 7.07362523 5.4262475
Pb 1.83359198 5.23863728 7.95865814
H 1.18440092 9.39987051 13.48571644
Pb 3.60998744 7.01941864 10.35492605
O 2.12810882 9.10464534 13.39528485
H 2.19259888 8.20359471 13.79560676
O -0.12270648 6.15632107 13.16220055
H 0.72912321 6.39997523 13.6173901
H 3.17671895 10.0839897 14.14276896
Pb 7.11353 3.55671 0.31755
Pb 7.11353 0.0 0.31755

Pb 5.33512 5.33512 2.8326
Pb 5.33512 1.77841 2.8326
Pb 5.35719749 1.71373031 7.96100302
H 6.74058766 2.90275054 13.6701641
Pb 7.11957727 -0.0374437 10.29179859
O 5.74301964 1.94123015 14.77329204
H 5.26266087 2.61823889 15.28338758
H 5.07159976 1.23356122 14.5763162
O 3.40935518 4.55745721 14.82353693
H 4.78673311 5.31080592 14.06310335
Pb 7.1703538 3.48753429 10.4748238
O 5.64227351 5.68856464 13.7018829
H 6.83104513 4.4483 13.46867354
Pb 7.11353 7.11353 0.31755
Pb 5.33512 8.89183 2.8326
Pb 5.3635104 8.82573925 7.97785511
Pb 7.1436203 10.6170072 5.39889828
Pb 3.5731384 7.07305405 5.43297112
Pb 5.37888516 5.27442716 7.9662869
H 5.85539737 8.97033276 13.31286259
O 5.98665765 8.80494477 14.26605909
H 5.69874245 6.59524198 14.06051974
Pb 7.18336033 7.02837155 10.36219587
H 5.24913148 9.29928795 14.69446808
O 2.36725477 6.48942853 14.27085384
C 2.47381723 5.41514801 14.92830279
Pb 8.89183 1.77841 2.8326
Pb 8.89183 5.33512 2.8326
Pb 8.91627257 1.70838082 7.93690544
Pb 7.14221818 3.51343779 5.43544342
Pb 10.70357919 3.40384338 10.30049737
Pb 10.66788627 -0.1047098 10.40916076
O 10.01876619 3.74650185 14.070972
O 8.08357724 0.20228605 14.86375124
H 10.64581421 3.0125311 14.24102446
H 9.1076801 3.42601298 13.87718978
O 7.31238348 3.59717801 13.24777045
H 7.47396807 0.95297362 15.02212055
Pb 8.89183 8.89183 2.8326
Pb 8.92822457 8.82094468 7.99126876
Pb 10.69326571 10.63091982 5.43507574
Pb 7.14221746 7.07585688 5.41611179
Pb 8.93757804 5.25657138 7.95222378
Pb 10.77115589 6.93952964 10.36443469
O 10.16567714 9.96590562 13.23461622
H 7.92745931 7.77264837 13.93110584
H 7.47339878 10.12721703 14.71645454

H 9.63225922 10.55215746 13.82750688
H 9.5733436 9.16185047 13.17630031
H 9.24578677 7.09311978 13.31135734
O 8.52521587 7.78554132 13.16181822

Configuration 3:
85
Lattice="10.6877079379 0.0 0.0 0.0 10.6790508945 0.0 0.0 0.0 35.2100018514" Properties=species:S:1:pos:R:3
Pb 3.55671 0.0 0.31755
Pb 0.0 0.0 0.31755
Pb 3.55671 3.55671 0.31755
Pb 0.0 3.55671 0.31755
Pb 1.77841 5.33512 2.8326
Pb 1.77841 1.77841 2.8326
Pb 1.74285639 1.72845774 7.95818517
Pb -0.0318315 3.53529487 5.40453444
Pb -0.02824624 -0.02283411 5.41494109
Pb 3.51357127 3.53451174 5.42186745
O 1.77119194 2.52882573 15.76113
Pb 3.53659026 3.49670308 10.33305318
H 2.32841776 1.7244075 15.87798049
O 0.53608508 4.48986785 13.04559151
H 2.32226894 3.17030627 15.25469837
H 1.5004013 4.48144058 13.31587462
O 3.09952814 4.39386779 14.01231479
Pb -0.06052576 -0.0683689 10.46304656
H 3.19410589 -0.26409985 16.94644635
H 0.12577514 3.70825216 13.4996524
Pb 0.0 7.11353 0.31755
Pb 3.55671 7.11353 0.31755
Pb 1.77841 8.89183 2.8326
Pb 1.72288512 8.8598074 7.96349515
Pb 3.52512655 7.10011331 5.42799201
Pb 1.73480846 5.30748937 7.96539055
H 2.70148359 9.74839772 14.66911621
H 2.65374868 8.38972268 13.8600653
Pb 3.43595564 7.03630274 10.40188918
O 2.44344601 9.34749602 13.80319516
H 0.86540105 9.77625538 13.45878752
Pb 3.46973334 10.60184603 10.35244034
O 3.47341222 6.61765714 13.74164129
C 3.64903574 5.50467957 14.316754
Pb 7.11353 3.55671 0.31755
Pb 7.11353 0.0 0.31755
Pb 5.33512 5.33512 2.8326
Pb 5.33512 1.77841 2.8326

Pb 5.30124228 1.73765838 7.98967745
O 5.49294641 2.54551094 13.71597947
H 7.13435746 5.87628221 12.99572116
H 4.64893626 3.01199947 13.90700269
H 5.40566007 1.62632816 14.05587267
Pb 7.11550396 3.52774634 10.31530277
H 6.97020579 3.20875502 14.48474197
O 3.25785132 0.11805588 16.05608407
Pb 7.11353 7.11353 0.31755
Pb 5.33512 8.89183 2.8326
Pb 5.25339128 8.87371788 7.97722269
Pb 7.09917084 7.09876585 5.41803254
Pb 5.27585803 5.29871329 7.9637741
Pb 3.51458706 10.66076019 5.41302362
H 6.40187488 7.46185179 14.40434139
O 5.67699075 8.12293186 14.51493973
O 7.51614055 6.09690724 13.8680486
Pb 7.00849614 7.10039852 10.24670031
H 4.8485649 7.6580135 14.22046435
Pb 7.09495377 10.65523781 10.30433479
H 4.23332553 10.78723165 15.80976821
O 5.71252287 10.67433407 15.03396818
H 5.75851776 9.68930295 14.76913487
H 7.65163587 5.1859755 14.31294017
H 4.37241801 5.47881102 15.16616258
Pb 8.89183 1.77841 2.8326
Pb 8.89183 5.33512 2.8326
Pb 8.88924358 1.75101036 7.9480075
Pb 7.09533664 3.53308932 5.4404955
O 10.17703683 2.21528467 14.37651837
Pb 10.69507843 3.55026307 10.38179631
H 10.98444449 2.24944166 14.97782218
H 6.50352067 0.16703012 15.57106463
H 8.54946307 3.13998588 14.72527329
O 7.74352014 3.68722656 14.88362909
H 10.18026229 1.31196742 13.99369884
Pb 8.89183 8.89183 2.8326
Pb 8.85482396 8.88817153 7.94557216
Pb 10.66043901 7.09617099 5.40202168
Pb 8.8560776 5.30756428 7.9542633
Pb 7.09949952 10.65943606 5.42150755
Pb 10.54747782 7.10577497 10.40724288
H 10.53848638 6.21870156 13.30714351
O 10.5948119 9.98094051 13.22445318
O 10.00345794 7.04465604 13.18196039
H 9.08560788 6.75540764 13.44623975
H 10.17713637 9.09622527 13.32832051

Configuration 4:
85
Lattice="10.6877079379 0.0 0.0 0.0 10.6790508945 0.0 0.0 0.0 35.2100018514"
Properties=species:S:1:pos:R:3
Pb 3.55671 0.0 0.31755
Pb 0.0 0.0 0.31755
Pb 3.55671 3.55671 0.31755
Pb 0.0 3.55671 0.31755
Pb 1.77841 5.33512 2.8326
Pb 1.77841 1.77841 2.8326
Pb 1.74490286 1.71551174 7.95698737
Pb 3.55474315 -0.03131466 5.4196868
H 3.02189289 3.35170139 14.58675373
H 1.67570487 2.79918954 14.01791631
O 2.65008973 2.61318893 14.03373418
H 3.06643435 0.88807639 13.69956485
O 3.71789198 4.91505834 15.13651702
H -0.35939455 3.37578088 13.11170048
H 1.89318474 5.75630212 15.39786229
H -0.60931098 2.48311442 14.3859169
C 2.96483595 5.9306654 15.15182675
O -0.13772148 3.3315893 14.06117707
Pb 0.0 7.11353 0.31755
Pb 3.55671 7.11353 0.31755
Pb 1.77841 8.89183 2.8326
Pb 1.76238196 8.85912675 7.97448201
Pb -0.02015238 10.65386986 5.41761345
Pb 1.78714363 5.30410904 7.96949675
H 2.17094652 8.18175759 14.80006948
H 1.28140207 9.30347216 15.52288757
O 3.26532172 10.65360682 13.35770951
H 2.58980892 10.07026268 13.80641962
O 1.52540749 8.96889943 14.64311681
Pb 7.11353 3.55671 0.31755
Pb 7.11353 0.0 0.31755
Pb 5.33512 5.33512 2.8326
Pb 5.33512 1.77841 2.8326
Pb 5.29463609 1.7489499 7.98118789
Pb 7.10190879 3.5262439 5.43027126
Pb 3.54637857 3.53298414 5.42302922
O 6.08392009 4.89221216 14.06496156
O 5.58046294 2.33369325 13.24442119
H 5.83372211 3.25313212 13.54059868
H 4.60789157 2.32298285 13.35276281
Pb 7.08680514 3.56064656 10.32215563

Pb 3.42810182 -0.04028947 10.53943876
H 5.19787717 5.00747924 14.56300205
Pb 3.51413236 3.50018154 10.3356126
H 6.3031394 1.23672036 14.51434676
O 6.79132381 0.70797989 15.19495507
Pb 7.11353 7.11353 0.31755
Pb 5.33512 8.89183 2.8326
Pb 5.31327227 8.89398767 7.9722109
Pb 3.54191384 7.10915735 5.40289638
Pb 7.09257386 7.11142168 5.44288175
Pb 5.32823715 5.33265419 7.96556266
Pb 7.02907903 10.67783605 10.32758983
H 6.02011016 5.49785456 13.30506775
Pb 7.16613254 7.13927517 10.45421494
H 7.1009314 8.17595419 13.60859344
Pb 3.59911786 7.11211425 10.32855081
O 5.47377652 8.82821702 14.21875032
H 4.86154286 8.13184233 14.56742764
H 4.86204246 9.50128097 13.84114752
O 3.31283186 7.1286103 14.90541834
H 6.4381226 10.47721428 15.12764493
Pb 8.89183 1.77841 2.8326
Pb 8.89183 5.33512 2.8326
Pb 8.85730376 1.72850344 7.95369394
Pb 10.67030868 3.53520471 5.42529639
Pb 7.10247342 -0.02423853 5.37524054
Pb 8.88978954 5.30967573 7.96031632
Pb 10.65416748 3.46463141 10.22719531
H 8.47841467 0.970161 15.01871842
H 9.65263116 0.34738822 14.18583948
O 9.45444021 1.07372076 14.82295213
Pb 8.89183 8.89183 2.8326
Pb 8.87840425 8.87409381 7.98391957
Pb 10.67317636 7.10766415 5.40722761
Pb 10.59010281 10.54717272 10.4851158
O 7.92816321 7.83241432 13.17956679
Pb 10.70586811 7.02289365 10.30346087
H 7.82676771 5.20554589 14.62856034
O 8.70706769 5.6488082 14.59315344
H 8.25293809 7.04460238 13.71279554
H 9.37306082 4.9310768 14.49336281
H 9.27736558 8.9530905 13.14718784
O 10.04662078 9.58771068 13.07125562
H 10.79812261 9.20277169 13.5972156

Configuration 5:
85

Lattice="10.6877079379 0.0 0.0 0.0 10.6790508945 0.0 0.0 0.0 35.2100018514" Properties=species:S:1:pos:R:3
Pb 3.55671 0.0 0.31755
Pb 0.0 0.0 0.31755
Pb 3.55671 3.55671 0.31755
Pb 0.0 3.55671 0.31755
Pb 1.77841 5.33512 2.8326
Pb 1.77841 1.77841 2.8326
Pb 1.82834644 1.83549703 8.00343716
Pb 3.57924808 3.59625149 5.44763324
Pb 0.03132142 0.03709748 5.4242701
H 2.57543795 1.66048009 13.97386285
O 2.06250809 2.21272341 13.33378059
Pb 0.0349782 3.66233163 10.31993964
Pb 3.6668113 0.0748328 10.31516611
Pb 0.08057553 0.02527744 10.32646879
H 2.45880691 3.12060568 13.39341848
Pb 3.60392499 3.72539894 10.40345459
H 0.42493515 2.09940828 13.85907498
Pb 0.0 7.11353 0.31755
Pb 3.55671 7.11353 0.31755
Pb 1.77841 8.89183 2.8326
Pb 1.8298853 8.94484468 7.9692653
Pb 0.02194716 7.15874809 5.42954396
Pb 3.57609967 7.1639627 5.4211078
Pb 3.56617096 10.71354145 5.40066911
Pb 1.8102076 5.4325774 7.96977784
Pb 0.05126182 7.18898038 10.48221974
O 2.08668253 8.88417765 14.41339586
H 0.51181275 7.78257235 13.82326592
H 2.63464448 9.69480788 14.50013363
H 3.16153161 5.63321611 14.81623783
H 0.50710057 9.83854499 15.54404232
O -0.26828713 7.34049485 13.42080234
H 2.72487681 8.18722521 14.11840084
Pb 7.11353 3.55671 0.31755
Pb 7.11353 0.0 0.31755
Pb 5.33512 5.33512 2.8326
Pb 5.33512 1.77841 2.8326
Pb 5.38329468 1.83280913 7.95214715
Pb 7.14883526 3.60517531 5.43178819
Pb 7.23947884 0.10281067 10.4277484
O 3.27972251 4.64913023 13.04438965
Pb 7.12307964 3.63877356 10.27445965
O 3.66862563 0.6208884 15.00018887
H 6.48943527 3.78858008 14.30670324
H 5.41376799 2.20816037 13.15894153

H 4.53545162 1.04538753 14.74118659
O 5.82526544 2.03247511 14.02767451
H 6.66923155 1.49894482 13.80517789
Pb 7.11353 7.11353 0.31755
Pb 5.33512 8.89183 2.8326
Pb 5.3832047 8.9691283 7.96434503
Pb 5.36896694 5.44024351 7.96838525
Pb 7.14225184 7.15243177 5.3832728
Pb 3.6093172 7.22722054 10.54551216
H 5.37841143 7.46459625 14.34387851
O 6.20947468 7.38112457 14.85494816
H 6.77403033 4.82654548 13.19171194
O 3.67001071 6.87005878 13.28579876
H 3.59931492 11.40431543 15.96411666
C 3.36752742 5.70854262 13.72310574
O 6.86902046 4.69292058 14.15534269
H 6.42465446 6.42230162 14.79693346
Pb 8.89183 1.77841 2.8326
Pb 8.89183 5.33512 2.8326
Pb 8.95763212 1.83226468 7.98618695
Pb 8.93390823 5.41892682 7.98404588
Pb 10.71725533 3.60474159 5.42524777
Pb 7.14082306 0.03625516 5.46851483
H 10.00777149 3.96057764 14.49656386
H 8.12037983 -0.18753014 13.70895952
H 8.81928917 1.24302867 13.55181359
O 7.99152375 0.72946278 13.31807868
O 9.71780882 4.90184509 14.44826063
H 8.7355524 4.84165602 14.42689258
H 10.32624179 1.31848593 14.9682302
O 10.21080769 2.03769335 14.28851639
Pb 8.89183 8.89183 2.8326
Pb 8.95530945 8.9414297 7.97753427
H 9.04794097 8.36967664 14.00220767
O 8.39206075 8.98191243 14.4290903
H 7.5829855 8.42818269 14.61739024
Pb 7.1471366 7.23010815 10.32087518
H 10.31340756 6.4360554 13.83564822
H 9.64918503 9.8759053 15.56377434
O 10.4440369 10.3953727 15.83225935

[1] K. Mathew, V. S. C. Kolluru, S. Mula, S. N. Steinmann, R. G. Hennig, J. Chem. Phys. 151, 234101 (2019).
[2] K. Mathew, R. Sundararaman, K. Letchworth-Weaver, T. A. Arias, R. G. Hennig, J. Chem. Phys. 140, 084106 (2014).
[3] P. Hirunsit, J. Phys. Chem. C. 117, 8262–8268 (2013).