

Supporting Information:

Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models

Joseph A. Gauthier,^{†,†} Stefan Ringe,^{‡,†} Colin F. Dickens,^{†,‡} Alejandro J. Garza,[¶]
Alexis T. Bell,[§] Martin Head-Gordon,^{||} Jens K. Nørskov,^{†,‡} and Karen Chan^{*,†,‡}

[†]*SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States*

[‡]*SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, United States*

[¶]*The Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, Berkeley California 94720, United States*

[§]*Department of Chemical and Biomolecular Engineering, University of California at Berkeley, Berkeley, California 94720, United States*

^{||}*Department of Chemistry, University of California at Berkeley, Berkeley, California 94720, United States*

E-mail: kchan@fysik.dtu.dk

Figure S1 below shows that using a symmetric or asymmetric cell gives a small effect on the energetics.

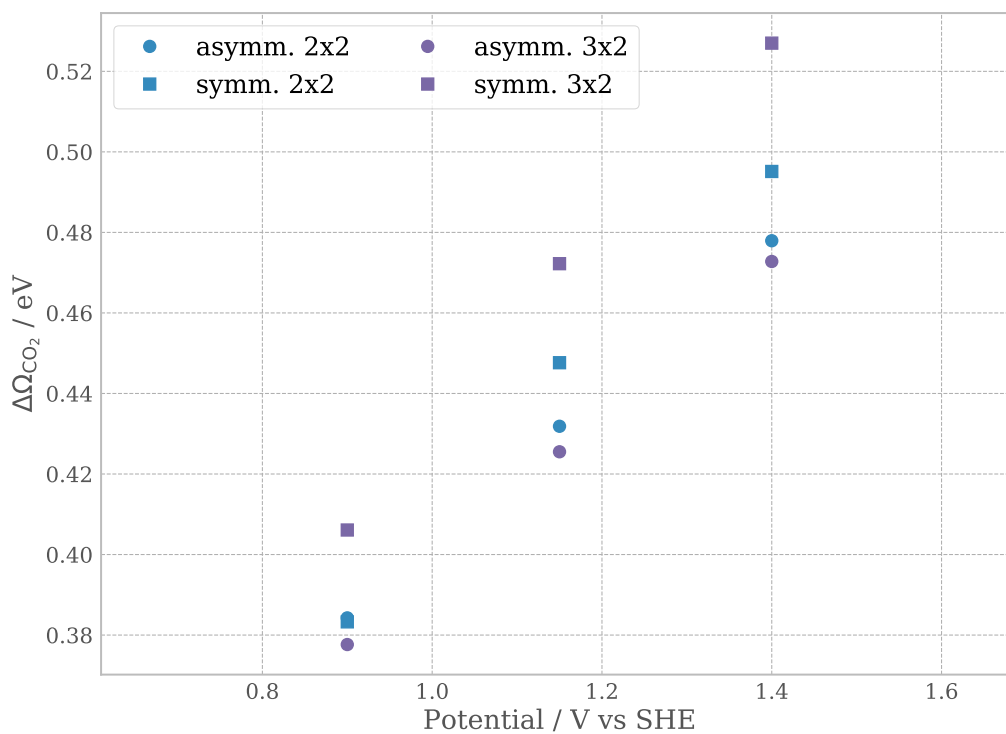


Figure S1: Ensemble corrected energies for CO₂ adsorption on Pt(111) for a symmetric and asymmetric (in the z-coordinate) slab.

As described in Section 1, there is a non-electrostatic contribution to the free energy of solvation calculated by many LPB/PCMs. This energy is written as Equation 5 in Section 1, where $\mathcal{S}$ is the surface area of the solvation cavity evaluated by integrating the gradient of the shape function. Figure S2 illustrates the numerical instability of this cavitation free energy term. In the left panel, we see the local electrostatic potential for a Pt(111) slab plotted as a planar average in the z -direction. Large numerical instabilities are observed in the interface region, with fluctuations on the order of several volts occurring in a short span along the z coordinate. In the vacuum region, small but consistent fluctuations occur, complicating the determination of a vacuum reference energy level. On the right, the adjustable parameter τ is set to 0, removing the numerical instabilities. For these reasons, τ is set to 0 for all calculations in this work, unless otherwise noted.

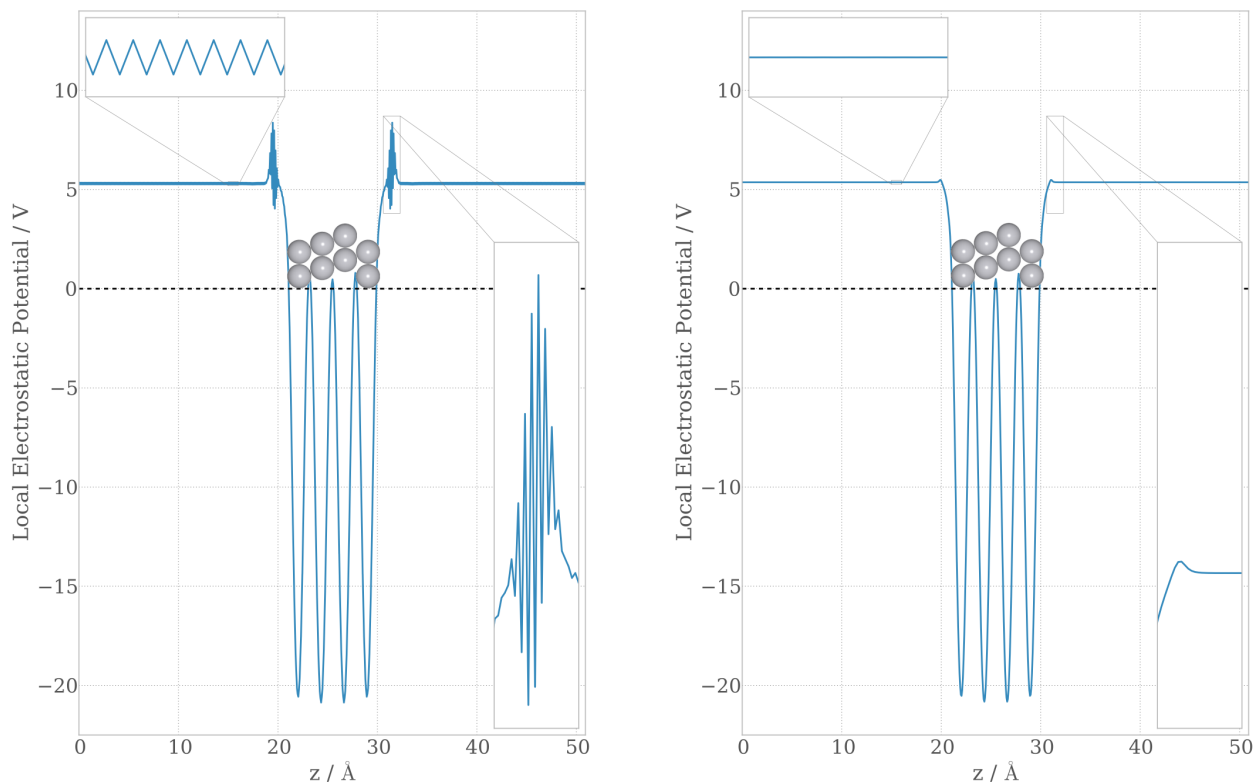


Figure S2: Left: Local electrostatic potential of a Pt(111) slab with τ set to the default value of $0.525 \text{ meV } \text{\AA}^{-2}$. Right: Local electrostatic potential of a clean Pt(111) slab with τ set to 0.

Figure S3 is a plot showing capacitance curves for a Pt(111) slab at two levels of dielectric

constant, effective surface tension, and electron density cutoff.

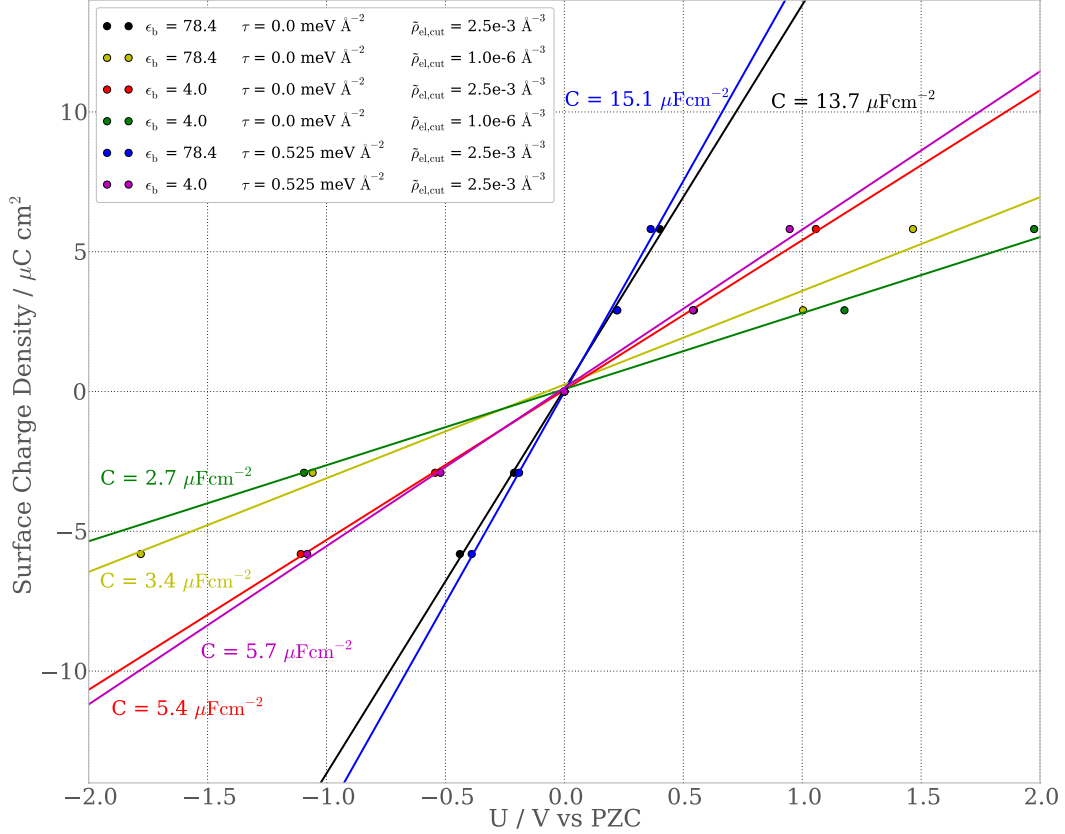


Figure S3: Observed decrease in capacitance and potential of zero charge of Pt(111) when PCM parameters are changed.

Shown in Figure S4 are the results of a full factorial experiment in several model parameters on the potential of zero charge (PZC) of Ag(100). Here, λ_D is the Debye length, ENCUT is the kinetic energy planewave cutoff, Vacuum is the amount of separation between periodic images (distance in both directions, so total separation is twice the value in the vacuum column), and TAU is the effective surface tension in the cavitation free energy term of the model (Eq. 5). The default value for λ_D is $1 * 10^{100} \text{ \AA}$, and the default value for τ is $0.525 \text{ meV \AA}^{-2}$. Experimental measurements of the PZC of Ag(100) are roughly -0.62 V vs SHE ,¹ which is reasonably reproduced for some values of the model parameters. Notably,

using $\lambda_D = 3\text{\AA}$ and the default effective surface tension τ gives a PZC of about -0.6 V vs SHE. However, using the default Debye length leads to drastically different predictions for the PZC.

$\lambda_0 / \text{\AA}$	ENCUT / eV	Vacuum / \AA	EDIFF / eV	TAU / meV \AA ²	PZC / V vs SHE
3	500	10	1e-4	0.0	-0.46
				0.525	-0.57
		50	1e-6	0.0	-0.46
				0.525	-0.57
			1e-4	0.0	-0.46
				0.525	-0.59
	800	10	1e-6	0.0	-0.46
				0.525	-0.56
		50	1e-4	0.0	-0.46
				0.525	-0.55
			1e-6	0.0	-0.46
				0.525	-0.54
1e100	500	10	1e-4	0.0	-7.84
				0.525	-7.91
		50	1e-6	0.0	-7.84
				0.525	-7.90
			1e-4	0.0	-2.47
				0.525	-2.57
	800	10	1e-6	0.0	-2.47
				0.525	-2.57
		50	1e-4	0.0	-7.96
				0.525	-8.01
			1e-6	0.0	-7.96
				0.525	-8.01
	800	10	1e-4	0.0	-2.49
				0.525	-2.57
		50	1e-6	0.0	-2.49
				0.525	-2.56
			1e-4	0.0	-2.49
				0.525	-2.56

Figure S4: Full factorial experiment illustrating the parameter dependence on the PZC of Ag(100)

Shown below is a parity plot between experimental² and calculated potentials of zero charge (PZC). Agreement is good for some of the surfaces shown, but Pt shows a significant disagreement.

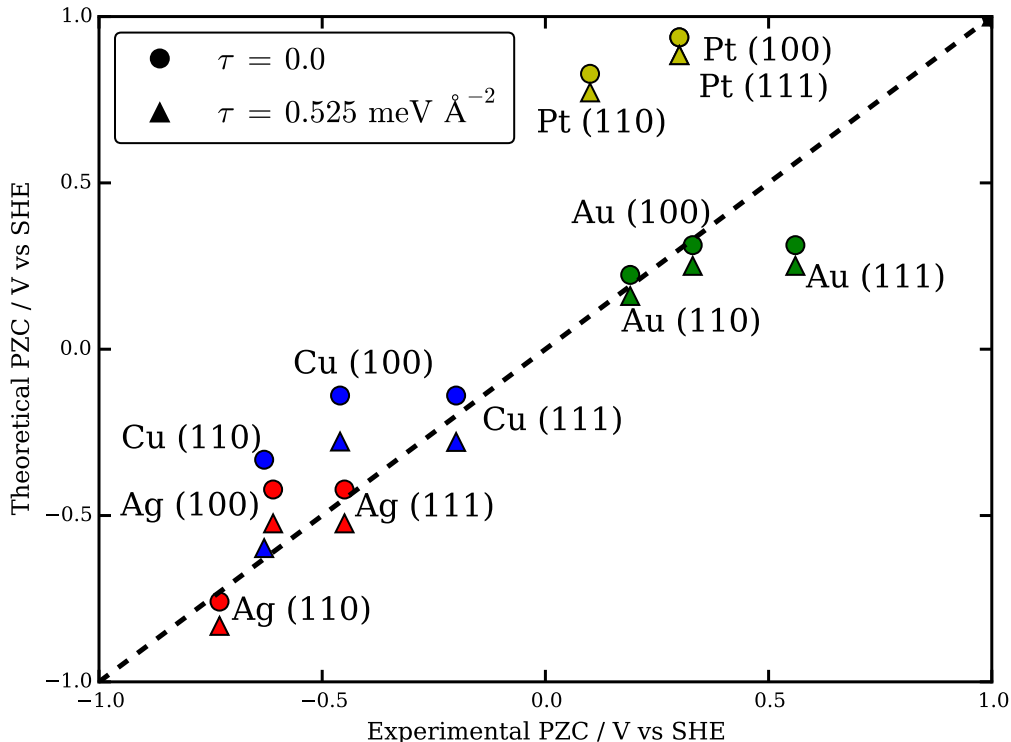


Figure S5: Parity plot between experimental² and calculated potentials of zero charge (PZC)

Figure S6 illustrates the convergence tests conducted to determine the spacing between periodic images in the calculations presented in this work. On the left, the adsorption energy of CO_2 is plotted as a function of the distance between periodic images, with each energy being calculated at a given potential. In this case, the potential is 1.15 V vs SHE. On the right is the same set of calculations, but instead plotted against inverse cell volume. The data being quite linear suggests the existence of a quadrupole effect, which in the current implementation of VASP can only be corrected for cubic unit cells. In principle, to achieve the infinite vacuum limit, one would need to do two calculations at smaller separation between slabs and extrapolate backwards. In this work, we approximate the infinite limit as 50 $\text{\AA}$

between periodic images.

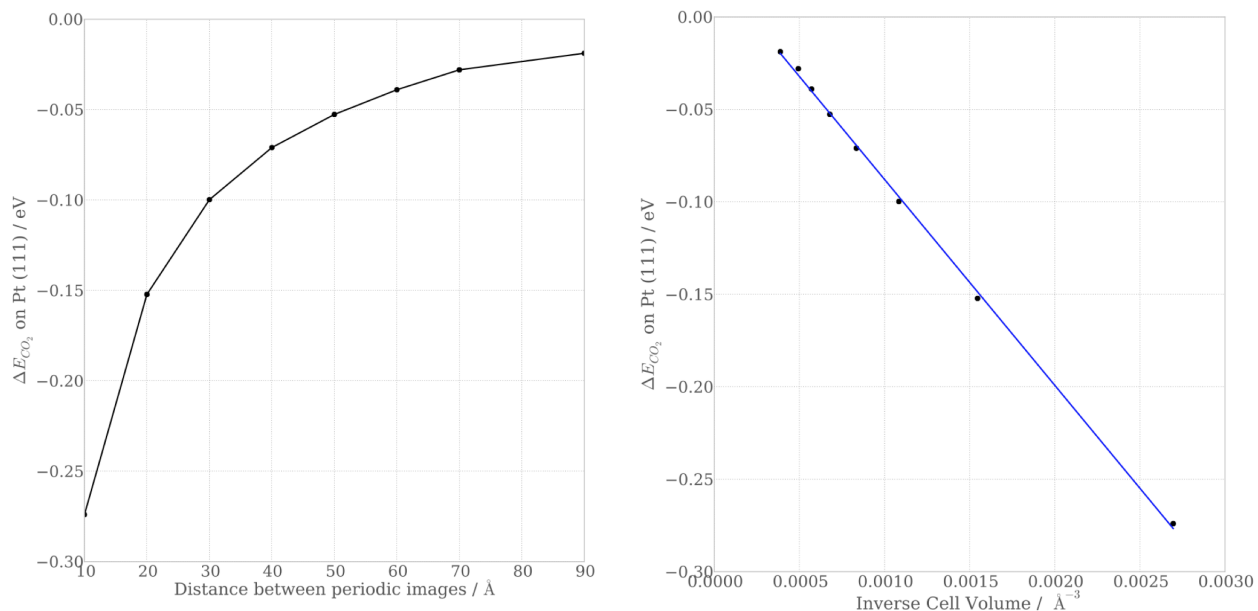


Figure S6: Convergence of CO₂ adsorption on Pt(111) with (left) distance between periodic images, and (right) inverse cell volume.

As noted in the text, the ramping parameter σ could in principle be used to adjust the rate at which the dielectric function increases to the bulk limit, possibly mitigating the issues outlined. Illustrated in Figure S7 is the dielectric function ramping to a bulk value of 78.4 for varying values of the ramping parameter, including the default value of 0.6. As can be seen, for values of σ lower than 0.6, the function approaches a square well. For values larger than 0.6, the ramping is indeed slower, but the ramping also has an earlier onset. For values much larger than 0.6, numerical instabilities are observed in both the slab and vacuum region

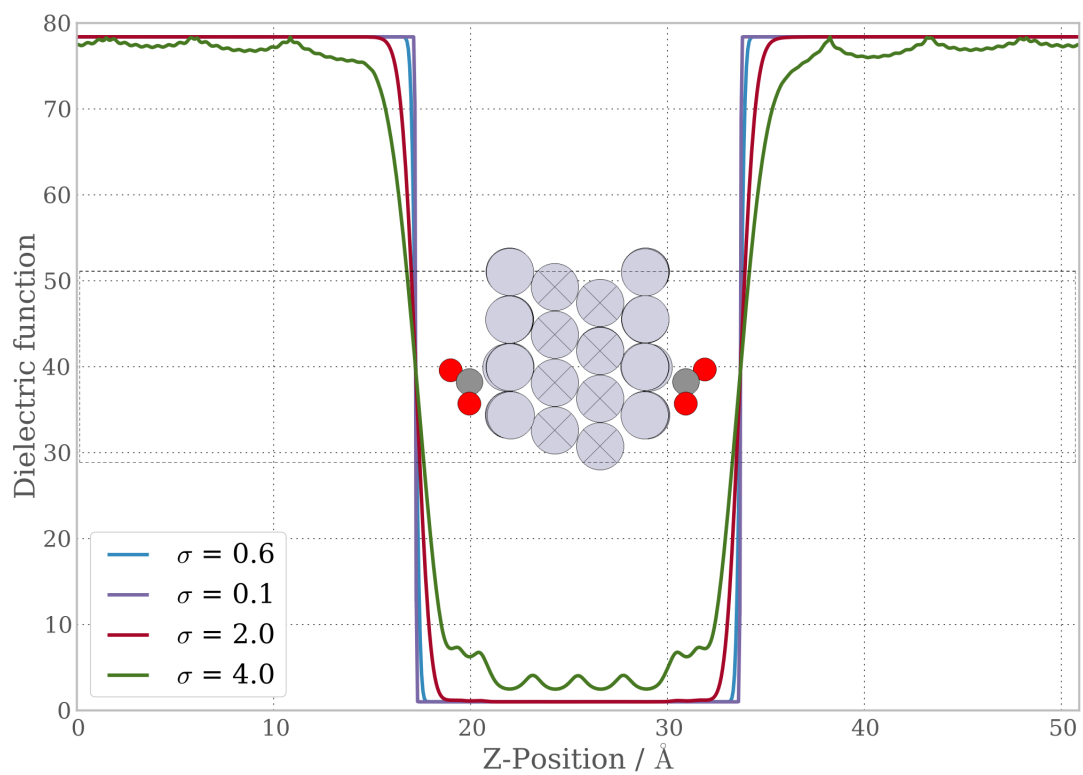


Figure S7: Planar average of dielectric function for varying values of the ramping parameter σ

Figure S8 illustrates that changing the Debye length λ_D does not significantly affect the overall interfacial capacitance. This is because the overall, measured interfacial capacitance is the result of two capacitances in series: the Helmholtz capacitance C_H , and the double layer capacitance C_{DL} . The measured capacitance is then:

$$C_{\text{total}} = \frac{1}{\frac{1}{C_H} + \frac{1}{C_{DL}}} \quad (1)$$

Most of the calculations in this work use $\lambda_D = 3.0 \text{ \AA}$, which corresponds to a bulk ion concentration of about 1 M. $\lambda_D = 9.6 \text{ \AA}$ corresponds to 0.1 M, and $\lambda_D = 30.4 \text{ \AA}$ corresponds to 0.01 M. As can be seen, decreasing the bulk ion concentration by one order of magnitude only results in a small overall change in the measured capacitance, an indication that at large ion concentrations, the Helmholtz capacitance dominates the measured capacitance.

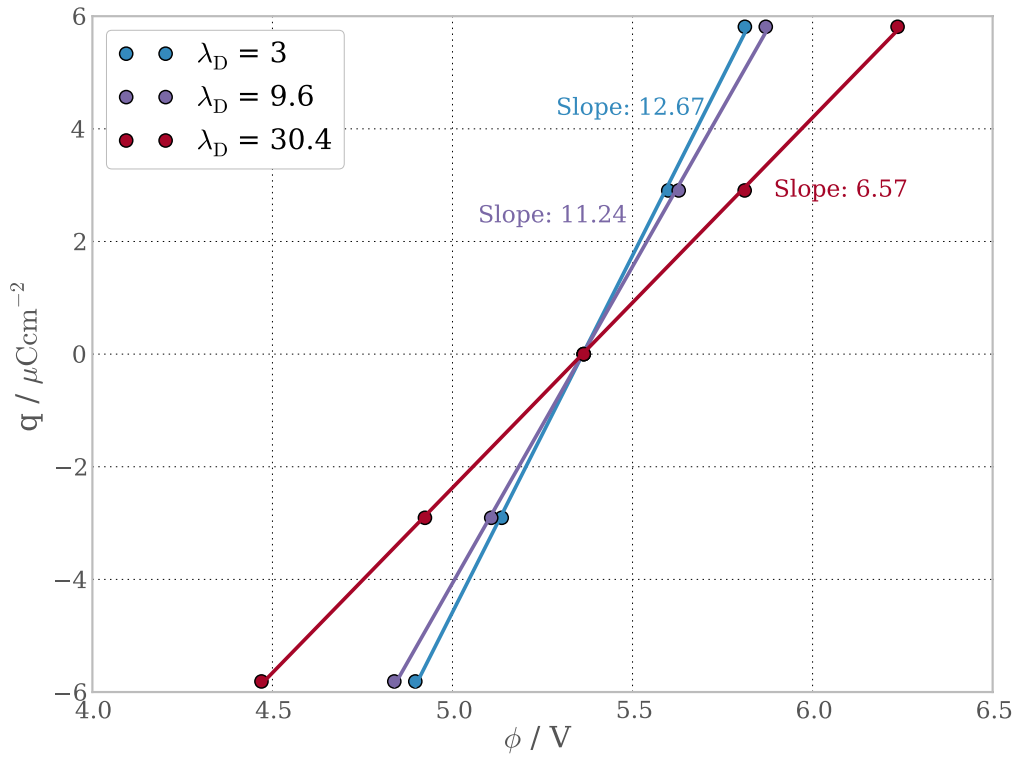
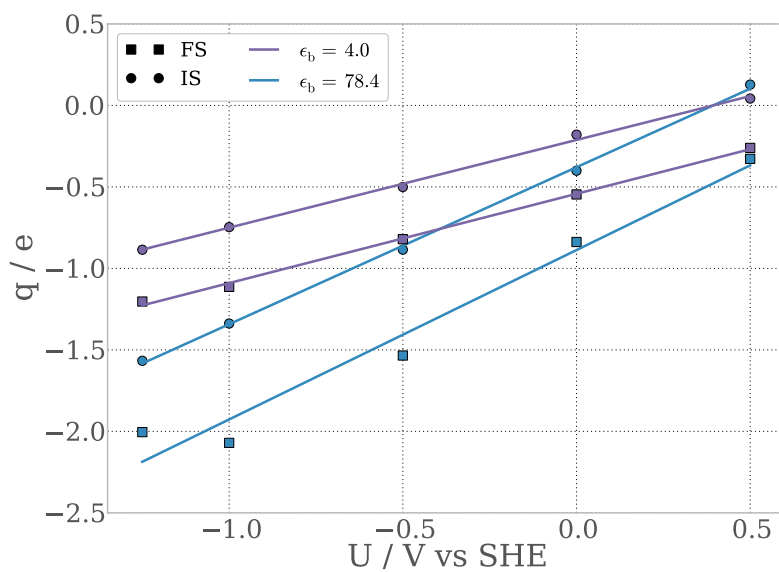
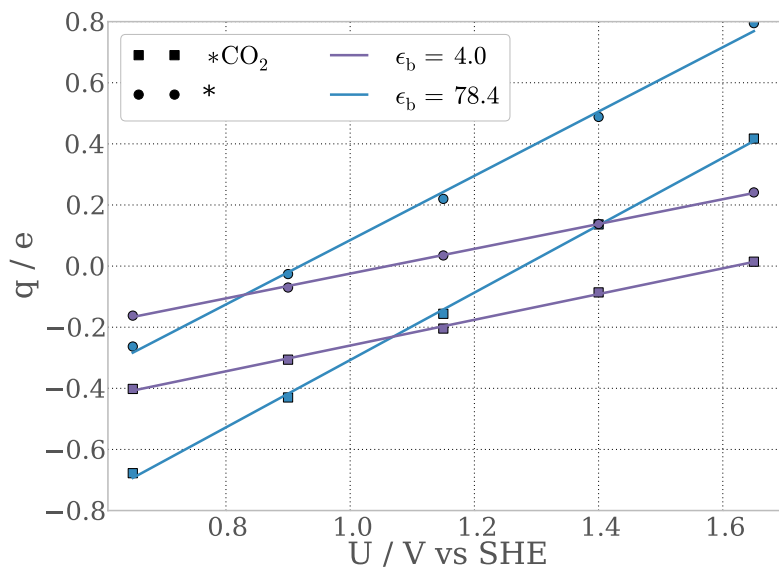


Figure S8: Measured interfacial capacitance of Pt (111) as a function of Debye length λ_D



(a)



(b)

Figure S9: (a) Charge vs potential curves for the initial and final states of the Volmer reaction on Pt(111). (b) Charge vs potential curves for the initial and final states of the CO₂ adsorption on Pt(111).

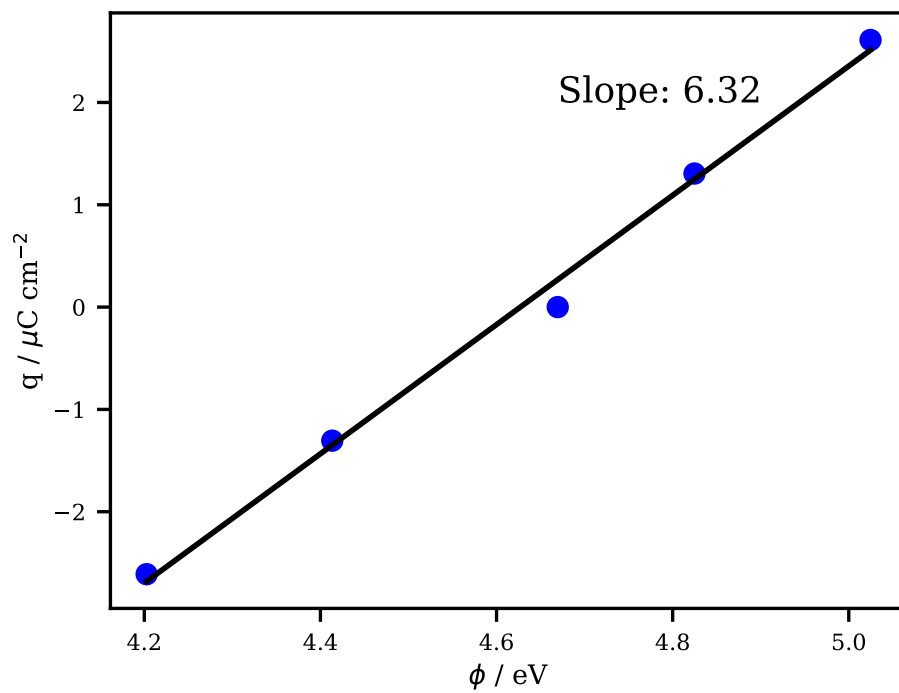


Figure S10: Surface charge density as a function of work function for Pt (111) with three layers of explicit solvent included.

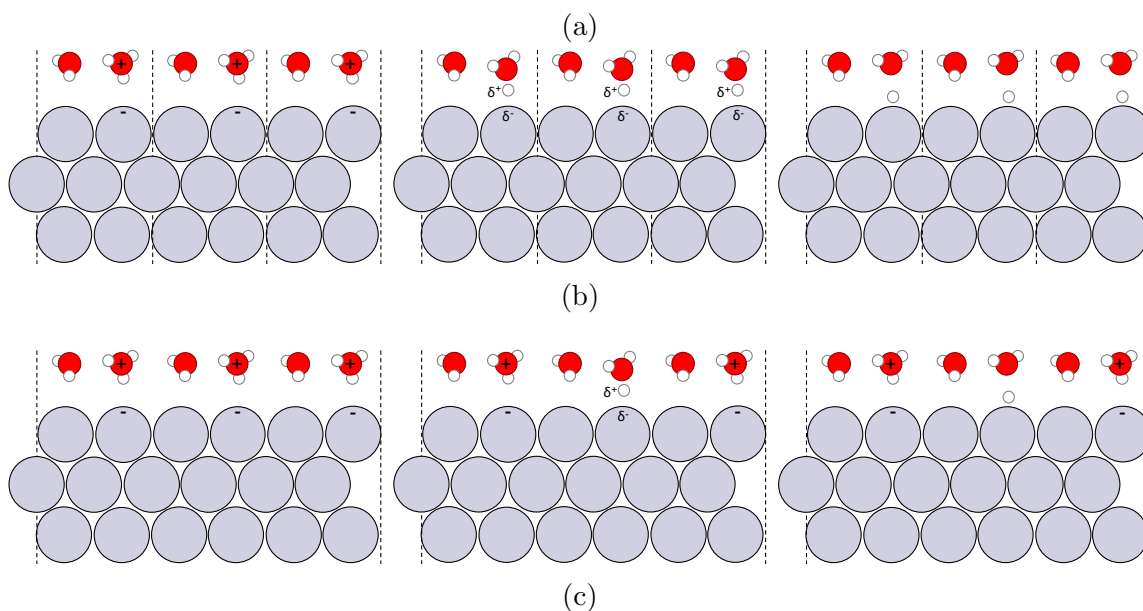
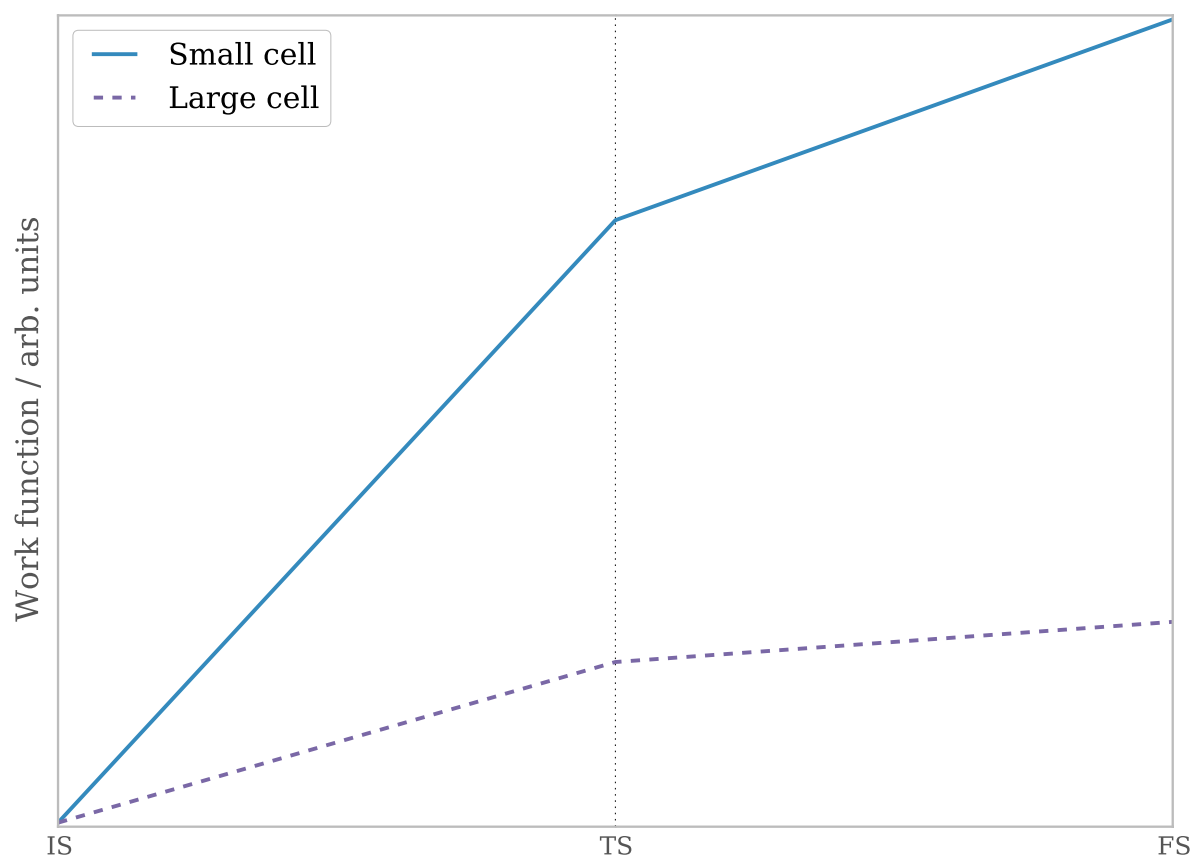


Figure S11: (a): Illustration of finite cell size effect during electrochemical (charge transfer) reactions. (b): Volmer reaction in a small unit cell results in a large work function change across the reaction coordinate. (c): Volmer reaction in a large unit cell results in a smaller work function change across the reaction coordinate.

Tables Corresponding to Figures in the Main Text

Figure 1 (a)

VASP geometry file (POSCAR):

C O Pt

1.0000000000000000

11.283231999999999 0.0000000000000000 0.0000000000000000

-2.8208080000000000 4.8857830000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 50.909539999999998

2 4 32

Selective dynamics

Cartesian

3.3820021099839996 2.4742973131240000 30.9985134487600007 T T T

3.3774267594080003 2.4669979533220001 19.9027282962199976 T T T

4.1629004926640008 2.5139161274710000 31.9368271804999999 T T T

2.0807690212000001 2.4489791856179997 30.9974952579600007 T T T

4.1560318251839998 2.4869026332640001 18.9622254542600004 T T T

2.0755759136720000 2.4501371161890000 19.9069537880399992 T T T

8.4007442122719986 4.8563999010380003 21.9919539987400015 T T T

1.4104068208080001 0.8142987952610000 24.3031962052000026 F F F

-0.0000028208079999 1.6285927047389999 26.6063437947999972 F F F

-0.0393023178639998 4.8368127969909995 28.8702401290599973 T T T

-0.0564443680799998 4.8416643795100001 22.0436780913800021 T T T

4.2312148208079998 0.8142987952610000 24.3031962052000026 F F F

2.8208051791919999 1.6285927047389999 26.6063437947999972 F F F

5.6339349398159992 0.0493415225170000 28.8676437425200021 T T T

5.6166687740480006 0.0457113857480000 22.0344634646399982 T T T

7.0520228208080002 0.8142987952610000 24.3031962052000026 F F F
 5.6416131791920003 1.6285927047389999 26.6063437947999972 F F F
 8.4345262088800013 0.0014168770700000 28.9229824124999979 T T T
 5.6074560151200004 4.8815128256579996 21.9705210824000012 T T T
 9.8728308208080016 0.8142987952610000 24.3031962052000026 F F F
 8.4624211791919990 1.6285927047389999 26.6063437947999972 F F F
 8.4097933643359983 4.8510646260020005 28.9360661642800032 T T T
 9.8091454385919992 2.4215699429880000 21.9837066532600005 T T T
 0.0000028208080001 3.2571902952610001 24.3031962052000026 F F F
 -1.4104068208079998 4.0714842047389999 26.6063437947999972 F F F
 1.3640778702159999 2.3949473114209998 28.9730264903199988 T T T
 1.3676659379920000 2.4459939722050001 21.9361571429000008 T T T
 2.8208108208080001 3.2571902952610001 24.3031962052000026 F F F
 1.4104011791920001 4.0714842047389999 26.6063437947999972 F F F
 4.1747845567679995 2.4455102796879999 29.0753037561799985 T T T
 4.1675548258639994 2.4508211258090000 21.8258361697199987 T T T
 5.6416188208080005 3.2571902952610001 24.3031962052000026 F F F
 4.2312091791919997 4.0714842047389999 26.6063437947999972 F F F
 7.0175779343200002 2.4448360416340003 28.9355061593399974 T T T
 6.9995275839280007 2.4540164278909997 21.9723029162999985 T T T
 8.4624268208080000 3.2571902952610001 24.3031962052000026 F F F
 7.0520171791919992 4.0714842047389999 26.6063437947999972 F F F
 9.8232410161679997 2.4125556733529998 28.9289388286799998 T T T

VASP input file (INCAR):

INCAR created by Atomic Simulation Environment

ENCUT = 500.000000

SIGMA = 0.050000

EDIFF = 0.0001

EDIFFG = -0.03

PREC = Accurate

GGA = RP

ALGO = Normal

ISPIN = 1

ISMEAR = 0

NELM = 250

NEDOS = 2001

LORBIT = 11

NSW = 0

IBRION = 2

NPAR = 4

LVHAR = .TRUE.

LVTOT = .FALSE.

ISTART = 1

LSOL = .TRUE.

LAMBDA_D_K = 3.0

TAU = 0

ICHARG = 0

NELECT = 352.201729555

LRHOION = .TRUE.

Figure 1(b)

VASP geometry file (POSCAR):

C O Pt

1.0000000000000000

11.283231999999999 0.0000000000000000 0.0000000000000000

-2.8208080000000000 4.8857830000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 50.909539999999998

2 4 32

Selective dynamics

Cartesian

3.3808625035519997 2.4746100032360001 31.0012625639200010 T T T

3.3761263669199999 2.4674327880089999 19.8999282715200003 T T T

4.1650273818960004 2.5150203144290000 31.9349944370599985 T T T

2.0804643739360000 2.4486860386380003 30.9956116049799988 T T T

4.1580289572479998 2.4880361349200002 18.9640072881600013 T T T

2.0751415092400003 2.4499905426990001 19.9088374410200011 T T T

8.4007301082320005 4.8561311829729998 21.9919539987400015 T T T

1.4104068208080001 0.8142987952610000 24.3031962052000026 F F F

-0.0000028208079999 1.6285927047389999 26.6063437947999972 F F F

-0.0394772079600000 4.8365098784449998 28.8703928576800024 T T T

-0.0564415472720003 4.8413858898790005 22.0434744532200000 T T T

4.2312148208079998 0.8142987952610000 24.3031962052000026 F F F

2.8208051791919999 1.6285927047389999 26.6063437947999972 F F F

5.6337008127520001 0.0489653172260000 28.8676946520599991 T T T

5.6166433867760004 0.0455403833430000 22.0342089169399991 T T T

7.0520228208080002 0.8142987952610000 24.3031962052000026 F F F

5.6416131791920003 1.6285927047389999 26.6063437947999972 F F F

8.4345487753440018 0.0010064712980000 28.9228805934200004 T T T
 5.6073544660320005 4.8812392218100005 21.9705719919399982 T T T
 9.8728308208080016 0.8142987952610000 24.3031962052000026 F F F
 8.4624211791919990 1.6285927047389999 26.6063437947999972 F F F
 8.4097849019119995 4.8507665932389994 28.9359134356599981 T T T
 9.8091144097039997 2.4213696258850002 21.9837066532600005 T T T
 0.0000028208080001 3.2571902952610001 24.3031962052000026 F F F
 -1.4104068208079998 4.0714842047389999 26.6063437947999972 F F F
 1.3642104481919999 2.3947176796200003 28.9742992288200014 T T T
 1.3677336373839999 2.4455444801689996 21.9348844044000018 T T T
 2.8208108208080001 3.2571902952610001 24.3031962052000026 F F F
 1.4104011791920001 4.0714842047389999 26.6063437947999972 F F F
 4.1752979438239999 2.4450901023499996 29.0740819272199964 T T T
 4.1679582014080001 2.4505524077440000 21.8270579986800008 T T T
 5.6416188208080005 3.2571902952610001 24.3031962052000026 F F F
 4.2312091791919997 4.0714842047389999 26.6063437947999972 F F F
 7.0174509979600010 2.4444696079089998 28.9354043402599999 T T T
 6.9994429596880003 2.4537525956090001 21.9723029162999985 T T T
 8.4624268208080000 3.2571902952610001 24.3031962052000026 F F F
 7.0520171791919992 4.0714842047389999 26.6063437947999972 F F F
 9.8231846000080001 2.4122234401089999 28.9288879191399992 T T T

VASP input file (INCAR):

INCAR created by Atomic Simulation Environment

ENCUT = 500.000000

SIGMA = 0.050000

EDIFF = 0.0001

EDIFFG = -0.03

PREC = Accurate

GGA = RP

ALGO = Normal

ISPIN = 1

ISMEAR = 0

NELM = 250

NEDOS = 2001

LORBIT = 11

NSW = 0

IBRION = 2

NPAR = 4

LVHAR = .TRUE.

ISTART = 1

LSOL = .TRUE.

LAMBDA_D_K = 3.0

TAU = 0

ICHARG = 0

NELECT = 352.201729555

NC_K_IONS= 1e-6

LRHOION = .TRUE.

Figure 2

Table corresponding to data in Figure 2:

z-axis	$\varepsilon, \varepsilon_b = 78.4$	$\varepsilon, \varepsilon_b = 4.0$	$\rho_{\text{ion}}, \varepsilon_b = 78.4$	$\rho_{\text{ion}}, \varepsilon_b = 4.0$
0.0	78.4	4.0	4.7314263e-10	3.8187061e-10
0.0673	78.4	4.0	4.7340808e-10	3.8204875e-10
0.1347	78.4	4.0	4.7368009e-10	3.8240009e-10
0.202	78.4	4.0	4.7442826e-10	3.8295424e-10
0.2694	78.4	4.0	4.7518394e-10	3.8368207e-10
0.3367	78.4	4.0	4.7641676e-10	3.8461634e-10
0.404	78.4	4.0	4.7765773e-10	3.8572909e-10
0.4714	78.4	4.0	4.7937644e-10	3.8705176e-10
0.5387	78.4	4.0	4.8110384e-10	3.8855336e-10
0.6061	78.4	4.0	4.833102e-10	3.9026246e-10
0.6734	78.4	4.0	4.8552691e-10	3.9214708e-10
0.7407	78.4	4.0	4.8822519e-10	3.9423738e-10
0.8081	78.4	4.0	4.9093653e-10	3.9650472e-10
0.8754	78.4	4.0	4.941325e-10	3.9898264e-10
0.9428	78.4	4.0	4.9734401e-10	4.016441e-10
1.0101	78.4	4.0	5.0104286e-10	4.0452172e-10
1.0775	78.4	4.0	5.0475954e-10	4.075856e-10
1.1448	78.4	4.0	5.0896679e-10	4.1086538e-10
1.2121	78.4	4.0	5.1319529e-10	4.1432977e-10
1.2795	78.4	4.0	5.1791899e-10	4.1800959e-10
1.3468	78.4	4.0	5.226685e-10	4.2187669e-10
1.4142	78.4	4.0	5.2791847e-10	4.2596546e-10
1.4815	78.4	4.0	5.331987e-10	4.3024976e-10
1.5488	78.4	4.0	5.3898433e-10	4.3476353e-10

1.6162	78.4	4.0	5.4480448e-10	4.39478e-10
1.6835	78.4	4.0	5.5113542e-10	4.4442401e-10
1.7509	78.4	4.0	5.5750616e-10	4.49571e-10
1.8182	78.4	4.0	5.6439454e-10	4.5495062e-10
1.8855	78.4	4.0	5.713293e-10	4.6053525e-10
1.9529	78.4	4.0	5.7878933e-10	4.6636021e-10
2.0202	78.4	4.0	5.8630236e-10	4.7240028e-10
2.0876	78.4	4.0	5.9434804e-10	4.7869077e-10
2.1549	78.4	4.0	6.0245311e-10	4.8520411e-10
2.2222	78.4	4.0	6.1109862e-10	4.9197252e-10
2.2896	78.4	4.0	6.1981094e-10	4.9896629e-10
2.3569	78.4	4.0	6.2907298e-10	5.0621802e-10
2.4243	78.4	4.0	6.3841065e-10	5.1370068e-10
2.4916	78.4	4.0	6.4830831e-10	5.2145062e-10
2.5589	78.4	4.0	6.5829065e-10	5.2944355e-10
2.6263	78.4	4.0	6.6884308e-10	5.3771633e-10
2.6936	78.4	4.0	6.7948902e-10	5.4624263e-10
2.761	78.4	4.0	6.9071555e-10	5.5505621e-10
2.8283	78.4	4.0	7.0204543e-10	5.6412834e-10
2.8956	78.4	4.0	7.1396794e-10	5.7349276e-10
2.963	78.4	4.0	7.2600516e-10	5.8312308e-10
3.0303	78.4	4.0	7.3864824e-10	5.9305683e-10
3.0977	78.4	4.0	7.5141784e-10	6.032707e-10
3.165	78.4	4.0	7.6480651e-10	6.1380321e-10
3.2324	78.4	4.0	7.7833334e-10	6.2462937e-10
3.2997	78.4	4.0	7.9249281e-10	6.3578471e-10
3.367	78.4	4.0	8.0680307e-10	6.4724155e-10

3.4344	78.4	4.0	8.2176116e-10	6.5903501e-10
3.5017	78.4	4.0	8.3688437e-10	6.7113944e-10
3.5691	78.4	4.0	8.5267201e-10	6.8359373e-10
3.6364	78.4	4.0	8.6863972e-10	6.9637556e-10
3.7037	78.4	4.0	8.8528862e-10	7.0952532e-10
3.7711	78.4	4.0	9.0213249e-10	7.2301943e-10
3.8384	78.4	4.0	9.1967469e-10	7.3689544e-10
3.9058	78.4	4.0	9.3742777e-10	7.511269e-10
3.9731	78.4	4.0	9.5589803e-10	7.6575053e-10
4.0404	78.4	4.0	9.745969e-10	7.8074155e-10
4.1078	78.4	4.0	9.940334e-10	7.9614036e-10
4.1751	78.4	4.0	1.0137172e-09	8.119258e-10
4.2425	78.4	4.0	1.0341594e-09	8.2814028e-10
4.3098	78.4	4.0	1.0548676e-09	8.4476179e-10
4.3771	78.4	4.0	1.0763556e-09	8.6183012e-10
4.4445	78.4	4.0	1.0981292e-09	8.7932024e-10
4.5118	78.4	4.0	1.1207057e-09	8.9727076e-10
4.5792	78.4	4.0	1.1435896e-09	9.1565792e-10
4.6465	78.4	4.0	1.1673013e-09	9.3452393e-10
4.7138	78.4	4.0	1.1913434e-09	9.5384885e-10
4.7812	78.4	4.0	1.2162388e-09	9.7367736e-10
4.8485	78.4	4.0	1.2414877e-09	9.9398919e-10
4.9159	78.4	4.0	1.2676161e-09	1.0148267e-09
4.9832	78.4	4.0	1.2941223e-09	1.0361665e-09
5.0505	78.4	4.0	1.3215359e-09	1.0580493e-09
5.1179	78.4	4.0	1.3493538e-09	1.0804528e-09
5.1852	78.4	4.0	1.3781093e-09	1.1034212e-09

5.2526	78.4	4.0	1.407297e-09	1.1269359e-09
5.3199	78.4	4.0	1.4374534e-09	1.1510442e-09
5.3873	78.4	4.0	1.4680704e-09	1.1757279e-09
5.4546	78.4	4.0	1.499688e-09	1.201032e-09
5.5219	78.4	4.0	1.5317956e-09	1.2269352e-09
5.5893	78.4	4.0	1.5649377e-09	1.253481e-09
5.6566	78.4	4.0	1.5986018e-09	1.2806482e-09
5.724	78.4	4.0	1.6333365e-09	1.3084838e-09
5.7913	78.4	4.0	1.6686272e-09	1.3369707e-09
5.8586	78.4	4.0	1.7050262e-09	1.3661593e-09
5.926	78.4	4.0	1.7420156e-09	1.3960332e-09
5.9933	78.4	4.0	1.7801518e-09	1.4266413e-09
6.0607	78.4	4.0	1.8189143e-09	1.4579642e-09
6.128	78.4	4.0	1.8588642e-09	1.4900485e-09
6.1953	78.4	4.0	1.899479e-09	1.5228751e-09
6.2627	78.4	4.0	1.9413246e-09	1.5564937e-09
6.33	78.4	4.0	1.9838759e-09	1.5908892e-09
6.3974	78.4	4.0	2.0277033e-09	1.6261155e-09
6.4647	78.4	4.0	2.0722782e-09	1.6621587e-09
6.532	78.4	4.0	2.1181754e-09	1.6990714e-09
6.5994	78.4	4.0	2.1648635e-09	1.7368372e-09
6.6667	78.4	4.0	2.2129228e-09	1.7755061e-09
6.7341	78.4	4.0	2.2618192e-09	1.8150615e-09
6.8014	78.4	4.0	2.3121387e-09	1.8555565e-09
6.8687	78.4	4.0	2.3633445e-09	1.8969785e-09
6.9361	78.4	4.0	2.4160274e-09	1.939385e-09
7.0034	78.4	4.0	2.4696471e-09	1.9827655e-09

7.0708	78.4	4.0	2.5247996e-09	2.027177e-09
7.1381	78.4	4.0	2.5809411e-09	2.072606e-09
7.2055	78.4	4.0	2.6386738e-09	2.1191074e-09
7.2728	78.4	4.0	2.697451e-09	2.1666671e-09
7.3401	78.4	4.0	2.7578814e-09	2.2153425e-09
7.4075	78.4	4.0	2.8194151e-09	2.2651239e-09
7.4748	78.4	4.0	2.8826667e-09	2.3160735e-09
7.5422	78.4	4.0	2.9470825e-09	2.3681842e-09
7.6095	78.4	4.0	3.0132827e-09	2.4215184e-09
7.6768	78.4	4.0	3.0807101e-09	2.4760665e-09
7.7442	78.4	4.0	3.1499916e-09	2.5318885e-09
7.8115	78.4	4.0	3.2205668e-09	2.5889739e-09
7.8789	78.4	4.0	3.29307e-09	2.6473852e-09
7.9462	78.4	4.0	3.3669374e-09	2.7071163e-09
8.0135	78.4	4.0	3.4428102e-09	2.7682349e-09
8.0809	78.4	4.0	3.5201201e-09	2.8307381e-09
8.1482	78.4	4.0	3.5995151e-09	2.8946944e-09
8.2156	78.4	4.0	3.6804228e-09	2.960099e-09
8.2829	78.4	4.0	3.763499e-09	3.0270182e-09
8.3502	78.4	4.0	3.8481676e-09	3.0954459e-09
8.4176	78.4	4.0	3.9350927e-09	3.1654506e-09
8.4849	78.4	4.0	4.0236946e-09	3.2370307e-09
8.5523	78.4	4.0	4.1146451e-09	3.3102604e-09
8.6196	78.4	4.0	4.2073602e-09	3.3851419e-09
8.6869	78.4	4.0	4.3025192e-09	3.4617511e-09
8.7543	78.4	4.0	4.3995335e-09	3.5400889e-09
8.8216	78.4	4.0	4.4990913e-09	3.6202288e-09

8.889	78.4	4.0	4.6005998e-09	3.7021706e-09
8.9563	78.4	4.0	4.7047568e-09	3.7859899e-09
9.0236	78.4	4.0	4.8109655e-09	3.8716906e-09
9.091	78.4	4.0	4.9199325e-09	3.9593547e-09
9.1583	78.4	4.0	5.0310565e-09	4.0489906e-09
9.2257	78.4	4.0	5.1450527e-09	4.140683e-09
9.293	78.4	4.0	5.2613149e-09	4.2344393e-09
9.3604	78.4	4.0	5.3805681e-09	4.3303424e-09
9.4277	78.4	4.0	5.5022016e-09	4.4283986e-09
9.495	78.4	4.0	5.6269514e-09	4.5286924e-09
9.5624	78.4	4.0	5.7542022e-09	4.6312345e-09
9.6297	78.4	4.0	5.8847005e-09	4.7361161e-09
9.6971	78.4	4.0	6.0178259e-09	4.8433534e-09
9.7644	78.4	4.0	6.154335e-09	4.953041e-09
9.8317	78.4	4.0	6.2936019e-09	5.0651949e-09
9.8991	78.4	4.0	6.4363945e-09	5.1799087e-09
9.9664	78.4	4.0	6.582082e-09	5.2971967e-09
10.0338	78.4	4.0	6.7314444e-09	5.4171544e-09
10.1011	78.4	4.0	6.8838463e-09	5.5398007e-09
10.1684	78.4	4.0	7.0400798e-09	5.6652381e-09
10.2358	78.4	4.0	7.1995037e-09	5.7934916e-09
10.3031	78.4	4.0	7.3629222e-09	5.9246684e-09
10.3705	78.4	4.0	7.5296878e-09	6.0587942e-09
10.4378	78.4	4.0	7.7006177e-09	6.1959755e-09
10.5051	78.4	4.0	7.8750591e-09	6.3362369e-09
10.5725	78.4	4.0	8.0538429e-09	6.4796866e-09
10.6398	78.4	4.0	8.2363113e-09	6.6263537e-09

10.7072	78.4	4.0	8.4233091e-09	6.7763541e-09
10.7745	78.4	4.0	8.6141725e-09	6.9297238e-09
10.8418	78.4	4.0	8.8097601e-09	7.0865845e-09
10.9092	78.4	4.0	9.0094013e-09	7.2469741e-09
10.9765	78.4	4.0	9.2139697e-09	7.4110144e-09
11.0439	78.4	4.0	9.4227886e-09	7.5787422e-09
11.1112	78.4	4.0	9.6367475e-09	7.7502813e-09
11.1785	78.4	4.0	9.8551642e-09	7.9256731e-09
11.2459	78.4	4.0	1.0078944e-08	8.1050495e-09
11.3132	78.4	4.0	1.0307399e-08	8.28846e-09
11.3806	78.4	4.0	1.054145e-08	8.4760435e-09
11.4479	78.4	4.0	1.0780402e-08	8.6678523e-09
11.5153	78.4	4.0	1.1025192e-08	8.8640266e-09
11.5826	78.4	4.0	1.1275119e-08	9.0646181e-09
11.6499	78.4	4.0	1.153114e-08	9.2697691e-09
11.7173	78.4	4.0	1.1792545e-08	9.4795362e-09
11.7846	78.4	4.0	1.206031e-08	9.6940704e-09
11.852	78.4	4.0	1.233372e-08	9.9134371e-09
11.9193	78.4	4.0	1.2613769e-08	1.0137796e-08
11.9866	78.4	4.0	1.2899734e-08	1.0367217e-08
12.054	78.4	4.0	1.3192628e-08	1.0601861e-08
12.1213	78.4	4.0	1.349172e-08	1.0841799e-08
12.1887	78.4	4.0	1.3798046e-08	1.1087196e-08
12.256	78.4	4.0	1.4110868e-08	1.1338125e-08
12.3233	78.4	4.0	1.4431242e-08	1.1594761e-08
12.3907	78.4	4.0	1.4758424e-08	1.1857188e-08
12.458	78.4	4.0	1.5093492e-08	1.2125591e-08

12.5254	78.4	4.0	1.5435692e-08	1.240006e-08
12.5927	78.4	4.0	1.5786125e-08	1.2680784e-08
12.66	78.4	4.0	1.614403e-08	1.2967853e-08
12.7274	78.4	4.0	1.6510533e-08	1.3261458e-08
12.7947	78.4	4.0	1.6884863e-08	1.3561697e-08
12.8621	78.4	4.0	1.7268172e-08	1.3868771e-08
12.9294	78.4	4.0	1.7659682e-08	1.4182787e-08
12.9967	78.4	4.0	1.8060571e-08	1.4503959e-08
13.0641	78.4	4.0	1.847005e-08	1.4832402e-08
13.1314	78.4	4.0	1.8889323e-08	1.5168336e-08
13.1988	78.4	4.0	1.9317593e-08	1.5511876e-08
13.2661	78.4	4.0	1.9756093e-08	1.5863247e-08
13.3335	78.4	4.0	2.0204017e-08	1.6222571e-08
13.4008	78.4	4.0	2.0662627e-08	1.6590083e-08
13.4681	78.4	4.0	2.1131108e-08	1.6965917e-08
13.5355	78.4	4.0	2.1610753e-08	1.7350323e-08
13.6028	78.4	4.0	2.2100736e-08	1.7743445e-08
13.6702	78.4	4.0	2.260238e-08	1.8145538e-08
13.7375	78.4	4.0	2.311485e-08	1.855675e-08
13.8048	78.4	4.0	2.3639503e-08	1.8977343e-08
13.8722	78.4	4.0	2.4175492e-08	1.9407471e-08
13.9395	78.4	4.0	2.472421e-08	1.9847408e-08
14.0069	78.4	4.0	2.52848e-08	2.0297321e-08
14.0742	78.4	4.0	2.5858691e-08	2.0757499e-08
14.1415	78.4	4.0	2.6445012e-08	2.1228124e-08
14.2089	78.4	4.0	2.704523e-08	2.1709494e-08
14.2762	78.4	4.0	2.7658462e-08	2.2201794e-08

14.3436	78.4	4.0	2.8286213e-08	2.2705329e-08
14.4109	78.4	4.0	2.8927591e-08	2.3220292e-08
14.4782	78.4	4.0	2.9584141e-08	2.3747001e-08
14.5456	78.4	4.0	3.0254958e-08	2.4285666e-08
14.6129	78.4	4.0	3.0941629e-08	2.4836622e-08
14.6803	78.4	4.0	3.1643235e-08	2.5400092e-08
14.7476	78.4	4.0	3.2361408e-08	2.5976425e-08
14.8149	78.4	4.0	3.3095211e-08	2.6565849e-08
14.8823	78.4	4.0	3.3846325e-08	2.7168722e-08
14.9496	78.4	4.0	3.4613798e-08	2.778528e-08
15.017	78.4	4.0	3.5399358e-08	2.8415895e-08
15.0843	78.4	4.0	3.6202039e-08	2.9060819e-08
15.1516	78.4	4.0	3.7023619e-08	2.9720444e-08
15.219	78.4	4.0	3.7863109e-08	3.039504e-08
15.2863	78.4	4.0	3.8722342e-08	3.1085009e-08
15.3537	78.4	4.0	3.9600307e-08	3.1790629e-08
15.421	78.4	4.0	4.0498889e-08	3.2512312e-08
15.4884	78.4	4.0	4.1417057e-08	3.3250338e-08
15.5557	78.4	4.0	4.2356749e-08	3.4005134e-08
15.623	78.4	4.0	4.3316908e-08	3.4776995e-08
15.6904	78.4	4.0	4.4299529e-08	3.5566364e-08
15.7577	78.4	4.0	4.5303519e-08	3.6373545e-08
15.8251	78.4	4.0	4.6330928e-08	3.719899e-08
15.8924	78.4	4.0	4.738062e-08	3.8043002e-08
15.9597	78.3999999996	3.99999999998	4.8454697e-08	3.8906027e-08
16.0271	78.3999999956	3.99999999983	4.9551973e-08	3.9788358e-08
16.0944	78.3999999584	3.99999999839	5.0674595e-08	4.0690432e-08

16.1618	78.3999996416	3.99999998611	5.1821306e-08	4.161253e-08
16.2291	78.3999972074	3.99999989176	5.2994286e-08	4.2555072e-08
16.2964	78.3999805236	3.9999992451	5.4192155e-08	4.35183e-08
16.3638	78.3998794019	3.99999532566	5.5416991e-08	4.4502543e-08
16.4311	78.3993393972	3.99997439524	5.6666815e-08	4.5507772e-08
16.4985	78.3967976702	3.99987587869	5.7942091e-08	4.6533462e-08
16.5658	78.3862347706	3.99946646398	5.923592e-08	4.7577001e-08
16.6331	78.3474670278	3.99796383829	6.053722e-08	4.8631057e-08
16.7005	78.2221103978	3.99310505418	6.1816491e-08	4.9678463e-08
16.7678	77.8664242359	3.97931876883	6.3030073e-08	5.0687507e-08
16.8352	76.9840424898	3.94511792596	6.4116505e-08	5.1611984e-08
16.9025	75.0735230084	3.87106678327	6.5020922e-08	5.2400364e-08
16.9698	71.4632909693	3.73113530889	6.5706759e-08	5.301327e-08
17.0372	65.506137961	3.50023790547	6.6178263e-08	5.3439109e-08
17.1045	56.9252811405	3.16764655583	6.6469078e-08	5.369934e-08
17.1719	46.1558065824	2.75022506133	6.6633189e-08	5.3837488e-08
17.2392	34.4168384997	2.29522629844	6.6714548e-08	5.3901685e-08
17.3065	23.3433275805	1.86602044886	6.6744555e-08	5.3929089e-08
17.3739	14.3310959362	1.51670914481	6.6738614e-08	5.3941117e-08
17.4412	8.01941662052	1.27207041165	6.6710407e-08	5.3945031e-08
17.5086	4.22717570083	1.12508432949	6.666161e-08	5.3940504e-08
17.5759	2.28158292886	1.04967375693	6.6587425e-08	5.3921143e-08
17.6433	1.434938204	1.01685806992	6.6473714e-08	5.3878392e-08
17.7106	1.12493699471	1.00484251917	6.6305693e-08	5.3799204e-08
17.7779	1.03015272295	1.00116871019	6.6066556e-08	5.3671422e-08
17.8453	1.00608440899	1.00023582981	6.5746639e-08	5.3483119e-08
17.9126	1.00102300019	1.00003965117	6.5341704e-08	5.3230005e-08

17.98	1.00014275765	1.00000553324	6.4861385e-08	5.2914875e-08
18.0473	1.00001644365	1.00000063735	6.4320706e-08	5.2550352e-08
18.1146	1.00000155458	1.00000006025	6.3743873e-08	5.2153694e-08
18.182	1.00000012059	1.00000000467	6.3147573e-08	5.1742286e-08
18.2493	1.00000000778	1.00000000003	6.2546767e-08	5.1327914e-08
18.3167	1.00000000043	1.00000000002	6.1943654e-08	5.0915686e-08
18.384	1.00000000002	1.0	6.1341978e-08	5.0505236e-08
18.4513	1.0	1.0	6.0735996e-08	5.0093404e-08
18.5187	1.0	1.0	6.012356e-08	4.9675204e-08
18.586	1.0	1.0	5.9493733e-08	4.9244445e-08
18.6534	1.0	1.0	5.8839456e-08	4.8792578e-08
18.7207	1.0	1.0	5.8141567e-08	4.8307099e-08
18.788	1.0	1.0	5.7378055e-08	4.7767207e-08
18.8554	1.0	1.0	5.6501517e-08	4.7137329e-08
18.9227	1.0	1.0	5.5442374e-08	4.635653e-08
18.9901	1.0	1.0	5.4081251e-08	4.5327481e-08
19.0574	1.0	1.0	5.2256999e-08	4.3908023e-08
19.1247	1.0	1.0	4.9760976e-08	4.1919288e-08
19.1921	1.0	1.0	4.6390982e-08	3.9178001e-08
19.2594	1.0	1.0	4.2004958e-08	3.5560121e-08
19.3268	1.0	1.0	3.6613543e-08	3.1070068e-08
19.3941	1.0	1.0	3.0416539e-08	2.5889719e-08
19.4615	1.0	1.0	2.3806704e-08	2.0370184e-08
19.5288	1.0	1.0	1.7287169e-08	1.4971418e-08
19.5961	1.0	1.0	1.1367503e-08	1.0155078e-08
19.6635	1.0	1.0	6.4401919e-09	6.2706402e-09
19.7308	1.0	1.0	2.713113e-09	3.4672731e-09

19.7982	1.0	1.0	2.0586941e-10	1.6782947e-09
19.8655	1.0	1.0	1.1896512e-09	6.8286838e-10
19.9328	1.0	1.0	1.6724927e-09	2.1047901e-10
20.0002	1.0	1.0	1.5365791e-09	2.8041388e-11
20.0675	1.0	1.0	1.1186626e-09	2.1468276e-11
20.1349	1.0	1.0	6.8252778e-10	2.3370454e-11
20.2022	1.0	1.0	3.5876638e-10	1.4700957e-11
20.2695	1.0	1.0	1.6587596e-10	7.3622109e-12
20.3369	1.0	1.0	6.8709027e-11	3.1839944e-12
20.4042	1.0	1.0	2.5908043e-11	1.2323175e-12
20.4716	1.0	1.0	9.0182241e-12	4.3580055e-13
20.5389	1.0	1.0	2.9337536e-12	1.4268824e-13
20.6062	1.0	1.0	9.0210958e-13	4.3130923e-14
20.6736	1.0	1.0	2.6465261e-13	1.0823491e-14
20.7409	1.0	1.0	7.4262143e-14	9.3156455e-16
20.8083	1.0	1.0	1.9200961e-14	5.6672203e-17
20.8756	1.0	1.0	3.2469033e-15	0.0
20.9429	1.0	1.0	2.1767153e-16	0.0
21.0103	1.0	1.0	1.3828522e-17	0.0
21.0776	1.0	1.0	0.0	0.0
21.145	1.0	1.0	0.0	0.0
21.2123	1.0	1.0	0.0	0.0
21.2796	1.0	1.0	0.0	0.0
21.347	1.0	1.0	0.0	0.0
21.4143	1.0	1.0	0.0	0.0
21.4817	1.0	1.0	0.0	0.0
21.549	1.0	1.0	0.0	0.0

21.6164	1.0	1.0	0.0	0.0
21.6837	1.0	1.0	0.0	0.0
21.751	1.0	1.0	0.0	0.0
21.8184	1.0	1.0	0.0	0.0
21.8857	1.0	1.0	0.0	0.0
21.9531	1.0	1.0	0.0	0.0
22.0204	1.0	1.0	0.0	0.0
22.0877	1.0	1.0	0.0	0.0
22.1551	1.0	1.0	0.0	0.0
22.2224	1.0	1.0	0.0	0.0
22.2898	1.0	1.0	0.0	0.0
22.3571	1.0	1.0	0.0	0.0
22.4244	1.0	1.0	0.0	0.0
22.4918	1.0	1.0	0.0	0.0
22.5591	1.0	1.0	0.0	0.0
22.6265	1.0	1.0	0.0	0.0
22.6938	1.0	1.0	0.0	0.0
22.7611	1.0	1.0	0.0	0.0
22.8285	1.0	1.0	0.0	0.0
22.8958	1.0	1.0	0.0	0.0
22.9632	1.0	1.0	0.0	0.0
23.0305	1.0	1.0	0.0	0.0
23.0978	1.0	1.0	0.0	0.0
23.1652	1.0	1.0	0.0	0.0
23.2325	1.0	1.0	0.0	0.0
23.2999	1.0	1.0	0.0	0.0
23.3672	1.0	1.0	0.0	0.0

23.4346	1.0	1.0	0.0	0.0
23.5019	1.0	1.0	0.0	0.0
23.5692	1.0	1.0	0.0	0.0
23.6366	1.0	1.0	0.0	0.0
23.7039	1.0	1.0	0.0	0.0
23.7713	1.0	1.0	0.0	0.0
23.8386	1.0	1.0	0.0	0.0
23.9059	1.0	1.0	0.0	0.0
23.9733	1.0	1.0	0.0	0.0
24.0406	1.0	1.0	0.0	0.0
24.108	1.0	1.0	0.0	0.0
24.1753	1.0	1.0	0.0	0.0
24.2426	1.0	1.0	0.0	0.0
24.31	1.0	1.0	0.0	0.0
24.3773	1.0	1.0	0.0	0.0
24.4447	1.0	1.0	0.0	0.0
24.512	1.0	1.0	0.0	0.0
24.5793	1.0	1.0	0.0	0.0
24.6467	1.0	1.0	0.0	0.0
24.714	1.0	1.0	0.0	0.0
24.7814	1.0	1.0	0.0	0.0
24.8487	1.0	1.0	0.0	0.0
24.916	1.0	1.0	0.0	0.0
24.9834	1.0	1.0	0.0	0.0
25.0507	1.0	1.0	0.0	0.0
25.1181	1.0	1.0	0.0	0.0
25.1854	1.0	1.0	0.0	0.0

25.2527	1.0	1.0	0.0	0.0
25.3201	1.0	1.0	0.0	0.0
25.3874	1.0	1.0	0.0	0.0
25.4548	1.0	1.0	0.0	0.0
25.5221	1.0	1.0	0.0	0.0
25.5895	1.0	1.0	0.0	0.0
25.6568	1.0	1.0	0.0	0.0
25.7241	1.0	1.0	0.0	0.0
25.7915	1.0	1.0	0.0	0.0
25.8588	1.0	1.0	0.0	0.0
25.9262	1.0	1.0	0.0	0.0
25.9935	1.0	1.0	0.0	0.0
26.0608	1.0	1.0	0.0	0.0
26.1282	1.0	1.0	0.0	0.0
26.1955	1.0	1.0	0.0	0.0
26.2629	1.0	1.0	0.0	0.0
26.3302	1.0	1.0	0.0	0.0
26.3975	1.0	1.0	0.0	0.0
26.4649	1.0	1.0	0.0	0.0
26.5322	1.0	1.0	0.0	0.0
26.5996	1.0	1.0	0.0	0.0
26.6669	1.0	1.0	0.0	0.0
26.7342	1.0	1.0	0.0	0.0
26.8016	1.0	1.0	0.0	0.0
26.8689	1.0	1.0	0.0	0.0
26.9363	1.0	1.0	0.0	0.0
27.0036	1.0	1.0	0.0	0.0

27.0709	1.0	1.0	0.0	0.0
27.1383	1.0	1.0	0.0	0.0
27.2056	1.0	1.0	0.0	0.0
27.273	1.0	1.0	0.0	0.0
27.3403	1.0	1.0	0.0	0.0
27.4076	1.0	1.0	0.0	0.0
27.475	1.0	1.0	0.0	0.0
27.5423	1.0	1.0	0.0	0.0
27.6097	1.0	1.0	0.0	0.0
27.677	1.0	1.0	0.0	0.0
27.7444	1.0	1.0	0.0	0.0
27.8117	1.0	1.0	0.0	0.0
27.879	1.0	1.0	0.0	0.0
27.9464	1.0	1.0	0.0	0.0
28.0137	1.0	1.0	0.0	0.0
28.0811	1.0	1.0	0.0	0.0
28.1484	1.0	1.0	0.0	0.0
28.2157	1.0	1.0	0.0	0.0
28.2831	1.0	1.0	0.0	0.0
28.3504	1.0	1.0	0.0	0.0
28.4178	1.0	1.0	0.0	0.0
28.4851	1.0	1.0	0.0	0.0
28.5524	1.0	1.0	0.0	0.0
28.6198	1.0	1.0	0.0	0.0
28.6871	1.0	1.0	0.0	0.0
28.7545	1.0	1.0	0.0	0.0
28.8218	1.0	1.0	0.0	0.0

28.8891	1.0	1.0	0.0	0.0
28.9565	1.0	1.0	0.0	0.0
29.0238	1.0	1.0	0.0	0.0
29.0912	1.0	1.0	0.0	0.0
29.1585	1.0	1.0	0.0	0.0
29.2258	1.0	1.0	0.0	0.0
29.2932	1.0	1.0	0.0	0.0
29.3605	1.0	1.0	0.0	0.0
29.4279	1.0	1.0	0.0	0.0
29.4952	1.0	1.0	0.0	0.0
29.5626	1.0	1.0	0.0	0.0
29.6299	1.0	1.0	0.0	0.0
29.6972	1.0	1.0	0.0	0.0
29.7646	1.0	1.0	0.0	0.0
29.8319	1.0	1.0	0.0	0.0
29.8993	1.0	1.0	6.0237957e-18	0.0
29.9666	1.0	1.0	2.0709153e-16	0.0
30.0339	1.0	1.0	3.1951341e-15	0.0
30.1013	1.0	1.0	1.9081565e-14	5.1919697e-17
30.1686	1.0	1.0	7.4026276e-14	9.1151598e-16
30.236	1.0	1.0	2.6420729e-13	1.0830957e-14
30.3033	1.0	1.0	9.0160418e-13	4.3164722e-14
30.3706	1.0	1.0	2.934332e-12	1.4286703e-13
30.438	1.0	1.0	9.024979e-12	4.365354e-13
30.5053	1.0	1.0	2.5938827e-11	1.2348335e-12
30.5727	1.0	1.0	6.8818031e-11	3.191492e-12
30.64	1.0	1.0	1.6620609e-10	7.3825386e-12

30.7073	1.0	1.0	3.5964337e-10	1.4751524e-11
30.7747	1.0	1.0	6.8458909e-10	2.3484398e-11
30.842	1.0	1.0	1.1229788e-09	2.1694958e-11
30.9094	1.0	1.0	1.5447078e-09	2.7657531e-11
30.9767	1.0	1.0	1.6865079e-09	2.0995827e-10
31.044	1.0	1.0	1.21231e-09	6.8238894e-10
31.1114	1.0	1.0	1.7089809e-10	1.6782636e-09
31.1787	1.0	1.0	2.6612227e-09	3.468286e-09
31.2461	1.0	1.0	6.3662115e-09	6.2733143e-09
31.3134	1.0	1.0	1.1266564e-08	1.0159834e-08
31.3807	1.0	1.0	1.7155765e-08	1.4978146e-08
31.4481	1.0	1.0	2.3643486e-08	2.0377605e-08
31.5154	1.0	1.0	3.0222631e-08	2.5894829e-08
31.5828	1.0	1.0	3.6392334e-08	3.1068684e-08
31.6501	1.0	1.0	4.1761524e-08	3.5548759e-08
31.7175	1.0	1.0	4.6131241e-08	3.9155722e-08
31.7848	1.0	1.0	4.9490815e-08	4.1887842e-08
31.8521	1.0	1.0	5.1981512e-08	4.3870358e-08
31.9195	1.0	1.0	5.3804336e-08	4.5286194e-08
31.9868	1.0	1.0	5.5166627e-08	4.6313382e-08
32.0542	1.0	1.0	5.622839e-08	4.709347e-08
32.1215	1.0	1.0	5.7108175e-08	4.7723501e-08
32.1888	1.0	1.0	5.7875117e-08	4.8264226e-08
32.2562	1.0	1.0	5.8576493e-08	4.8751108e-08
32.3235	1.0	1.0	5.9234325e-08	4.9204836e-08
32.3909	1.0	1.0	5.98678e-08	4.9637847e-08
32.4582	1.0	1.0	6.0483921e-08	5.005857e-08

32.5255	1.00000000002	1.0	6.1093491e-08	5.0473029e-08
32.5929	1.00000000039	1.00000000002	6.1698584e-08	5.0886064e-08
32.6602	1.00000000712	1.00000000028	6.2304964e-08	5.1300766e-08
32.7276	1.00000011089	1.00000000043	6.2909111e-08	5.171767e-08
32.7949	1.00000143809	1.00000005574	6.3509152e-08	5.2132025e-08
32.8622	1.00001530447	1.0000005932	6.409058e-08	5.2532495e-08
32.9296	1.00013365945	1.0000051806	6.4636893e-08	5.2901868e-08
32.9969	1.00096326212	1.00003733574	6.5123762e-08	5.3222715e-08
33.0643	1.00576071704	1.00022328361	6.5535796e-08	5.3481994e-08
33.1316	1.02870230427	1.00111249241	6.5862972e-08	5.3676447e-08
33.1989	1.1195525789	1.00463382089	6.6109158e-08	5.3809918e-08
33.2663	1.4183061736	1.01621341758	6.628362e-08	5.3893958e-08
33.3336	2.23851670632	1.0480045235	6.6402932e-08	5.3940645e-08
33.401	4.13279117195	1.12142601442	6.6481851e-08	5.3963266e-08
33.4683	7.84269662238	1.26522079932	6.6534804e-08	5.3970788e-08
33.5356	14.0462397014	1.50566820548	6.6566984e-08	5.3969894e-08
33.603	22.9461650987	1.85062655421	6.6577129e-08	5.3961045e-08
33.6703	33.9365203934	2.27660931757	6.6551748e-08	5.3937166e-08
33.7377	45.6506253878	2.73064439488	6.6475646e-08	5.3877262e-08
33.805	56.4617108338	3.14967871449	6.6317999e-08	5.3744745e-08
33.8724	65.1331970134	3.48578282998	6.6035472e-08	5.3491797e-08
33.9397	71.1990073472	3.72089175765	6.5574068e-08	5.3074599e-08
34.007	74.9079458059	3.86464906225	6.4899343e-08	5.2470742e-08
34.0744	76.892233668	3.9415594445	6.4005661e-08	5.1690553e-08
34.1417	77.8214224811	3.97757451477	6.2928473e-08	5.0772393e-08
34.2091	78.2026453527	3.99235059506	6.1722065e-08	4.9767473e-08
34.2764	78.340041996	3.99767604636	6.0448103e-08	4.8722365e-08

34.3437	78.3837316092	3.99936944222	5.9150706e-08	4.7669435e-08
34.4111	78.3960488854	3.99984685603	5.7859979e-08	4.6626382e-08
34.4784	78.3991397349	3.99996665639	5.6587351e-08	4.5600838e-08
34.5458	78.399831756	3.99999347892	5.5339975e-08	4.4595545e-08
34.6131	78.3999703178	3.99999884953	5.4117433e-08	4.3611078e-08
34.6804	78.3999952394	3.99999981548	5.2921776e-08	4.2647493e-08
34.7478	78.3999992984	3.99999997281	5.1750898e-08	4.1704477e-08
34.8151	78.3999999039	3.99999999628	5.0606217e-08	4.0781802e-08
34.8825	78.3999999877	3.99999999952	4.9485528e-08	3.9879057e-08
34.9498	78.3999999985	3.99999999994	4.8390118e-08	3.8995963e-08
35.0171	78.3999999998	3.99999999999	4.7317818e-08	3.8132078e-08
35.0845	78.4	4.0	4.626984e-08	3.7287104e-08
35.1518	78.4	4.0	4.5244064e-08	3.6460594e-08
35.2192	78.4	4.0	4.4241648e-08	3.5652251e-08
35.2865	78.4	4.0	4.3260524e-08	3.4861637e-08
35.3538	78.4	4.0	4.2301806e-08	3.4088457e-08
35.4212	78.4	4.0	4.1363483e-08	3.3332279e-08
35.4885	78.4	4.0	4.0446634e-08	3.259281e-08
35.5559	78.4	4.0	3.9549304e-08	3.1869622e-08
35.6232	78.4	4.0	3.8672544e-08	3.1162428e-08
35.6906	78.4	4.0	3.7814455e-08	3.0470815e-08
35.7579	78.4	4.0	3.6976064e-08	2.9794512e-08
35.8252	78.4	4.0	3.6155529e-08	2.9133125e-08
35.8926	78.4	4.0	3.5353851e-08	2.8486398e-08
35.9599	78.4	4.0	3.456924e-08	2.785395e-08
36.0273	78.4	4.0	3.380268e-08	2.723553e-08
36.0946	78.4	4.0	3.3052431e-08	2.6630765e-08

36.1619	78.4	4.0	3.2319458e-08	2.6039413e-08
36.2293	78.4	4.0	3.1602073e-08	2.5461118e-08
36.2966	78.4	4.0	3.0901225e-08	2.4895652e-08
36.364	78.4	4.0	3.0215271e-08	2.4342677e-08
36.4313	78.4	4.0	2.9545143e-08	2.3801983e-08
36.4986	78.4	4.0	2.8889246e-08	2.3273242e-08
36.566	78.4	4.0	2.8248496e-08	2.2756249e-08
36.6333	78.4	4.0	2.7621339e-08	2.2250685e-08
36.7007	78.4	4.0	2.700868e-08	2.1756353e-08
36.768	78.4	4.0	2.6409007e-08	2.1272944e-08
36.8353	78.4	4.0	2.5823211e-08	2.0800275e-08
36.9027	78.4	4.0	2.524982e-08	2.0338056e-08
36.97	78.4	4.0	2.4689712e-08	1.9886116e-08
37.0374	78.4	4.0	2.4141453e-08	1.9444177e-08
37.1047	78.4	4.0	2.3605908e-08	1.9012073e-08
37.172	78.4	4.0	2.3081679e-08	1.858953e-08
37.2394	78.4	4.0	2.2569621e-08	1.8176388e-08
37.3067	78.4	4.0	2.2068371e-08	1.7772384e-08
37.3741	78.4	4.0	2.1578773e-08	1.7377368e-08
37.4414	78.4	4.0	2.1099497e-08	1.6991093e-08
37.5087	78.4	4.0	2.0631377e-08	1.6613421e-08
37.5761	78.4	4.0	2.0173115e-08	1.6244114e-08
37.6434	78.4	4.0	1.9725532e-08	1.5883039e-08
37.7108	78.4	4.0	1.9287362e-08	1.5529963e-08
37.7781	78.4	4.0	1.8859417e-08	1.5184756e-08
37.8455	78.4	4.0	1.8440461e-08	1.4847191e-08
37.9128	78.4	4.0	1.8031295e-08	1.4517148e-08

37.9801	78.4	4.0	1.7630713e-08	1.4194414e-08
38.0475	78.4	4.0	1.7239507e-08	1.3878881e-08
38.1148	78.4	4.0	1.6856496e-08	1.3570343e-08
38.1822	78.4	4.0	1.6482463e-08	1.3268696e-08
38.2495	78.4	4.0	1.6116254e-08	1.2973738e-08
38.3168	78.4	4.0	1.5758642e-08	1.2685367e-08
38.3842	78.4	4.0	1.5408499e-08	1.2403386e-08
38.4515	78.4	4.0	1.5066591e-08	1.2127699e-08
38.5189	78.4	4.0	1.4731813e-08	1.1858123e-08
38.5862	78.4	4.0	1.4404923e-08	1.1594572e-08
38.6535	78.4	4.0	1.408484e-08	1.133687e-08
38.7209	78.4	4.0	1.3772311e-08	1.1084935e-08
38.7882	78.4	4.0	1.3466278e-08	1.0838593e-08
38.8556	78.4	4.0	1.3167482e-08	1.0597763e-08
38.9229	78.4	4.0	1.2874884e-08	1.0362274e-08
38.9902	78.4	4.0	1.258922e-08	1.0132051e-08
39.0576	78.4	4.0	1.2309473e-08	9.9069351e-09
39.1249	78.4	4.0	1.2036368e-08	9.6868596e-09
39.1923	78.4	4.0	1.1768909e-08	9.4716718e-09
39.2596	78.4	4.0	1.1507815e-08	9.2613097e-09
39.3269	78.4	4.0	1.1252107e-08	9.0556215e-09
39.3943	78.4	4.0	1.1002496e-08	8.854545e-09
39.4616	78.4	4.0	1.0758024e-08	8.6579311e-09
39.529	78.4	4.0	1.0519396e-08	8.4657224e-09
39.5963	78.4	4.0	1.028567e-08	8.2777783e-09
39.6636	78.4	4.0	1.0057544e-08	8.0940499e-09
39.731	78.4	4.0	9.8340958e-09	7.9144038e-09

39.7983	78.4	4.0	9.6160144e-09	7.7387942e-09
39.8657	78.4	4.0	9.4023925e-09	7.5670888e-09
39.933	78.4	4.0	9.1939144e-09	7.3992407e-09
40.0004	78.4	4.0	8.9896889e-09	7.235119e-09
40.0677	78.4	4.0	8.7903943e-09	7.0746806e-09
40.135	78.4	4.0	8.5951553e-09	6.9178019e-09
40.2024	78.4	4.0	8.404644e-09	6.7644473e-09
40.2697	78.4	4.0	8.2179993e-09	6.6145003e-09
40.3371	78.4	4.0	8.035887e-09	6.4679284e-09
40.4044	78.4	4.0	7.8574598e-09	6.3246157e-09
40.4717	78.4	4.0	7.6833776e-09	6.1845282e-09
40.5391	78.4	4.0	7.5128076e-09	6.0475506e-09
40.6064	78.4	4.0	7.3464042e-09	5.9136515e-09
40.6738	78.4	4.0	7.1833484e-09	5.7827217e-09
40.7411	78.4	4.0	7.024289e-09	5.6547368e-09
40.8084	78.4	4.0	6.8684197e-09	5.5295942e-09
40.8758	78.4	4.0	6.716383e-09	5.4072726e-09
40.9431	78.4	4.0	6.5673847e-09	5.2876702e-09
41.0105	78.4	4.0	6.422062e-09	5.1707637e-09
41.0778	78.4	4.0	6.2796329e-09	5.0564511e-09
41.1451	78.4	4.0	6.1407299e-09	4.9447107e-09
41.2125	78.4	4.0	6.0045832e-09	4.8354455e-09
41.2798	78.4	4.0	5.87182e-09	4.7286402e-09
41.3472	78.4	4.0	5.7416817e-09	4.6242043e-09
41.4145	78.4	4.0	5.6147897e-09	4.5221256e-09
41.4818	78.4	4.0	5.4903958e-09	4.4223142e-09
41.5492	78.4	4.0	5.3691165e-09	4.324756e-09

41.6165	78.4	4.0	5.2502144e-09	4.22936e-09
41.6839	78.4	4.0	5.1343015e-09	4.136113e-09
41.7512	78.4	4.0	5.020651e-09	4.0449282e-09
41.8186	78.4	4.0	4.9098705e-09	3.9557979e-09
41.8859	78.4	4.0	4.8012428e-09	3.8686414e-09
41.9532	78.4	4.0	4.6953702e-09	3.7834546e-09
42.0206	78.4	4.0	4.5915446e-09	3.7001574e-09
42.0879	78.4	4.0	4.4903635e-09	3.6187435e-09
42.1553	78.4	4.0	4.3911284e-09	3.5391316e-09
42.2226	78.4	4.0	4.2944327e-09	3.4613152e-09
42.2899	78.4	4.0	4.1995872e-09	3.3852162e-09
42.3573	78.4	4.0	4.1071814e-09	3.3108333e-09
42.4246	78.4	4.0	4.0165345e-09	3.2380943e-09
42.492	78.4	4.0	3.9282312e-09	3.1670013e-09
42.5593	78.4	4.0	3.8415984e-09	3.097483e-09
42.6266	78.4	4.0	3.7572165e-09	3.0295395e-09
42.694	78.4	4.0	3.6744208e-09	2.9630976e-09
42.7613	78.4	4.0	3.5937879e-09	2.8981568e-09
42.8287	78.4	4.0	3.5146614e-09	2.8346462e-09
42.896	78.4	4.0	3.4376143e-09	2.7725697e-09
42.9633	78.4	4.0	3.3619976e-09	2.7118623e-09
43.0307	78.4	4.0	3.2883799e-09	2.6525314e-09
43.098	78.4	4.0	3.2161191e-09	2.5945129e-09
43.1654	78.4	4.0	3.1457797e-09	2.5378125e-09
43.2327	78.4	4.0	3.0767267e-09	2.482364e-09
43.3	78.4	4.0	3.0095214e-09	2.4281715e-09
43.3674	78.4	4.0	2.9435361e-09	2.3751708e-09

43.4347	78.4	4.0	2.8793287e-09	2.3233698e-09
43.5021	78.4	4.0	2.8162782e-09	2.2727094e-09
43.5694	78.4	4.0	2.7549387e-09	2.2232015e-09
43.6367	78.4	4.0	2.6946949e-09	2.1747883e-09
43.7041	78.4	4.0	2.6360971e-09	2.1274799e-09
43.7714	78.4	4.0	2.5785363e-09	2.0812162e-09
43.8388	78.4	4.0	2.5225598e-09	2.0360056e-09
43.9061	78.4	4.0	2.4675651e-09	1.9917887e-09
43.9735	78.4	4.0	2.4140966e-09	1.9485774e-09
44.0408	78.4	4.0	2.3615576e-09	1.9063173e-09
44.1081	78.4	4.0	2.310489e-09	1.8650239e-09
44.1755	78.4	4.0	2.2602991e-09	1.8246448e-09
44.2428	78.4	4.0	2.2115254e-09	1.7851939e-09
44.3102	78.4	4.0	2.1635816e-09	1.7466163e-09
44.3775	78.4	4.0	2.1170025e-09	1.7089236e-09
44.4448	78.4	4.0	2.0712074e-09	1.6720612e-09
44.5122	78.4	4.0	2.0267286e-09	1.6360437e-09
44.5795	78.4	4.0	1.9829906e-09	1.6008208e-09
44.6469	78.4	4.0	1.9405226e-09	1.5664111e-09
44.7142	78.4	4.0	1.8987536e-09	1.5327664e-09
44.7815	78.4	4.0	1.8582093e-09	1.4999041e-09
44.8489	78.4	4.0	1.8183235e-09	1.4677734e-09
44.9162	78.4	4.0	1.7796194e-09	1.4363891e-09
44.9836	78.4	4.0	1.7415358e-09	1.4057001e-09
45.0509	78.4	4.0	1.7045938e-09	1.3757235e-09
45.1182	78.4	4.0	1.6682368e-09	1.3464125e-09
45.1856	78.4	4.0	1.632983e-09	1.3177879e-09

45.2529	78.4	4.0	1.5982797e-09	1.2898053e-09
45.3203	78.4	4.0	1.5646421e-09	1.2624848e-09
45.3876	78.4	4.0	1.5315215e-09	1.2357793e-09
45.4549	78.4	4.0	1.4994308e-09	1.2097061e-09
45.5223	78.4	4.0	1.4678258e-09	1.1842174e-09
45.5896	78.4	4.0	1.4372176e-09	1.159332e-09
45.657	78.4	4.0	1.4070658e-09	1.1350059e-09
45.7243	78.4	4.0	1.3778793e-09	1.111262e-09
45.7916	78.4	4.0	1.3491209e-09	1.0880588e-09
45.859	78.4	4.0	1.3212968e-09	1.0654186e-09
45.9263	78.4	4.0	1.2938733e-09	1.0432978e-09
45.9937	78.4	4.0	1.2673543e-09	1.0217155e-09
46.061	78.4	4.0	1.2412101e-09	1.0006267e-09
46.1284	78.4	4.0	1.2159432e-09	9.8005176e-10
46.1957	78.4	4.0	1.1910273e-09	9.5994895e-10
46.263	78.4	4.0	1.1669629e-09	9.4034259e-10
46.3304	78.4	4.0	1.1432264e-09	9.211938e-10
46.3977	78.4	4.0	1.1203159e-09	9.0252681e-10
46.4651	78.4	4.0	1.0977108e-09	8.8430058e-10
46.5324	78.4	4.0	1.0759071e-09	8.6653617e-10
46.5997	78.4	4.0	1.0543878e-09	8.4919074e-10
46.6671	78.4	4.0	1.0336474e-09	8.3228585e-10
46.7344	78.4	4.0	1.0131722e-09	8.1578176e-10
46.8018	78.4	4.0	9.9345502e-10	7.9970388e-10
46.8691	78.4	4.0	9.7398436e-10	7.8401544e-10
46.9364	78.4	4.0	9.5525094e-10	7.6874222e-10
47.0038	78.4	4.0	9.3674562e-10	7.5384551e-10

47.0711	78.4	4.0	9.1895749e-10	7.393479e-10
47.1385	78.4	4.0	9.013803e-10	7.252085e-10
47.2058	78.4	4.0	8.8450207e-10	7.1144986e-10
47.2731	78.4	4.0	8.6781936e-10	6.9803375e-10
47.3405	78.4	4.0	8.5181873e-10	6.8498647e-10
47.4078	78.4	4.0	8.3599879e-10	6.7227296e-10
47.4752	78.4	4.0	8.2084417e-10	6.599203e-10
47.5425	78.4	4.0	8.0585538e-10	6.4789179e-10
47.6098	78.4	4.0	7.915156e-10	6.3621133e-10
47.6772	78.4	4.0	7.7732781e-10	6.248397e-10
47.7445	78.4	4.0	7.6377435e-10	6.1380031e-10
47.8119	78.4	4.0	7.5036068e-10	6.0305613e-10
47.8792	78.4	4.0	7.3756798e-10	5.9263419e-10
47.9466	78.4	4.0	7.2490344e-10	5.8250078e-10
48.0139	78.4	4.0	7.1284655e-10	5.7268408e-10
48.0812	78.4	4.0	7.00906e-10	5.6314911e-10
48.1486	78.4	4.0	6.8956002e-10	5.5392095e-10
48.2159	78.4	4.0	6.7831935e-10	5.4496186e-10
48.2833	78.4	4.0	6.6766162e-10	5.3629597e-10
48.3506	78.4	4.0	6.5709972e-10	5.2788723e-10
48.4179	78.4	4.0	6.4711042e-10	5.1976321e-10
48.4853	78.4	4.0	6.3720803e-10	5.1189133e-10
48.5526	78.4	4.0	6.2786793e-10	5.0430072e-10
48.62	78.4	4.0	6.1860554e-10	4.9695786e-10
48.6873	78.4	4.0	6.0989517e-10	4.8988895e-10
48.7546	78.4	4.0	6.0125389e-10	4.8305753e-10
48.822	78.4	4.0	5.9315564e-10	4.764884e-10

48.8893	78.4	4.0	5.8511934e-10	4.7014636e-10
48.9567	78.4	4.0	5.7761835e-10	4.6405939e-10
49.024	78.4	4.0	5.7017275e-10	4.5819584e-10
49.0913	78.4	4.0	5.6325479e-10	4.5258565e-10
49.1587	78.4	4.0	5.5638532e-10	4.4719663e-10
49.226	78.4	4.0	5.500357e-10	4.4205602e-10
49.2934	78.4	4.0	5.4372807e-10	4.3712851e-10
49.3607	78.4	4.0	5.3793361e-10	4.3243957e-10
49.428	78.4	4.0	5.3217603e-10	4.2795472e-10
49.4954	78.4	4.0	5.2692626e-10	4.2370231e-10
49.5627	78.4	4.0	5.2170889e-10	4.1965147e-10
49.6301	78.4	4.0	5.1699399e-10	4.1583285e-10
49.6974	78.4	4.0	5.1230666e-10	4.1221546e-10
49.7647	78.4	4.0	5.0811627e-10	4.0882754e-10
49.8321	78.4	4.0	5.0394883e-10	4.0563491e-10
49.8994	78.4	4.0	5.0027377e-10	4.026637e-10
49.9668	78.4	4.0	4.9661836e-10	3.9988005e-10
50.0341	78.4	4.0	4.9345207e-10	3.9731271e-10
50.1015	78.4	4.0	4.9030285e-10	3.9493144e-10
50.1688	78.4	4.0	4.8763963e-10	3.9276762e-10
50.2361	78.4	4.0	4.8499053e-10	3.9079134e-10
50.3035	78.4	4.0	4.82824e-10	3.8903183e-10
50.3708	78.4	4.0	4.8066872e-10	3.87456e-10
50.4382	78.4	4.0	4.7899339e-10	3.8609069e-10
50.5055	78.4	4.0	4.7732772e-10	3.8490267e-10
50.5728	78.4	4.0	4.7614073e-10	3.8392108e-10
50.6402	78.4	4.0	4.749626e-10	3.8311625e-10

50.7075	78.4	4.0	4.7426208e-10	3.8252025e-10
50.7749	78.4	4.0	4.7356928e-10	3.8210416e-10
50.8422	78.4	4.0	4.7335269e-10	3.818983e-10
50.9095	78.4	4.0	4.7314263e-10	3.8187061e-10

Figure 3

VASP geometry file (POSCAR) for explicit solvent:

H Pt O Na

1.0000000000000000

8.4624236950871214 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.7715651967104353 0.0000000000000000

0.0000000000000000 0.0000000000000000 50.9095400134004095

14 36 7 1

Selective dynamics

Cartesian

1.0659759450930684 2.0250908735047140 32.1192630418971916 T T T

1.6831708172431104 2.3740752572930561 33.5040002890336552 T T T

6.8521660873114500 4.7278936976849453 31.4586970379684843 T T T

5.7215205044393924 4.0050325713046924 32.1970564026839838 T T T

7.3378099654725260 4.2564390946124000 33.9261613819480488 T T T

7.9179766067091331 2.8647539113062797 34.2252656966067335 T T T

1.0333670040649510 4.0769971056290677 34.8559052766626962 T T T

2.3462895507581871 3.9701488312127964 35.7172064843776411 T T T

2.7465469453780056 5.5213292433347583 33.8907643887056267 T T T

2.5582141677744188 7.0140257696063388 33.4287162922273637 T T T

1.5656961191737269 9.7024937136565796 32.9647008919980564 T T T

1.5692084401764581 8.6558812219265953 31.8159351439966755 T T T

3.8164571233234330 9.1301340758586456 32.5144917982712514 T T T

5.0135136645115681 9.4998130785993133 31.5947266533366928 T T T

1.4104039491811668 0.8142970997258927 24.3031800044668671 F F F

0.0000000000000000 1.6285941994517161 26.6063600089335424 F F F

2.8105894542994876 0.0145928730315068 28.9353067030616948 T T T

0.0000000000000000 3.2571883989035015 24.3031800044668671 F F F
 7.0520197459059544 4.0714854986293245 26.6063600089335424 F F F
 1.4013318673323105 2.4606179299554518 28.9407577537914129 T T T
 4.2312118475435607 0.8142970997258927 24.3031800044668671 F F F
 2.8208078983623937 1.6285941994517161 26.6063600089335424 F F F
 5.6306868003318424 0.0155729353225044 28.9321962653248193 T T T
 2.8208078983623937 3.2571883989035015 24.3031800044668671 F F F
 1.4104039491811668 4.0714854986293245 26.6063600089335424 F F F
 4.2201672924129783 2.4572535908943101 28.9416564309855211 T T T
 7.0520197459059544 0.8142970997258927 24.3031800044668671 F F F
 5.6416157967247278 1.6285941994517161 26.6063600089335424 F F F
 -0.0081013543551041 0.0141752624668891 28.9352932608552322 T T T
 5.6416157967247278 3.2571883989035015 24.3031800044668671 F F F
 4.2312118475435607 4.0714854986293245 26.6063600089335424 F F F
 7.0475690961844322 2.4566815926853729 28.9395987495579305 T T T
 1.4104039491811668 5.7000796980811108 24.3031800044668671 F F F
 0.0000000000000000 6.5143767978069338 26.6063600089335424 F F F
 2.8070057787247586 4.9046146621039606 28.9415195708459443 T T T
 0.0000000000000000 8.1429709972587201 24.3031800044668671 F F F
 7.0520197459059544 8.9572680969845422 26.6063600089335424 F F F
 1.4026734550921189 7.3472750863526963 28.9420445199767364 T T T
 4.2312118475435607 5.7000796980811108 24.3031800044668671 F F F
 2.8208078983623937 6.5143767978069338 26.6063600089335424 F F F
 5.6303877271612954 4.9032505399522730 28.9386467756992189 T T T
 2.8208078983623937 8.1429709972587201 24.3031800044668671 F F F
 1.4104039491811668 8.9572680969845422 26.6063600089335424 F F F
 4.2226917144217495 7.3456129161638026 28.9344226740872266 T T T

7.0520197459059544 5.7000796980811108 24.3031800044668671 F F F
 5.6416157967247278 6.5143767978069338 26.6063600089335424 F F F
 -0.0071934543003217 4.9024133052118799 28.9507785528253692 T T T
 5.6416157967247278 8.1429709972587201 24.3031800044668671 F F F
 4.2312118475435607 8.9572680969845422 26.6063600089335424 F F F
 7.0457955055801680 7.3473583044516486 28.9532254329039738 T T T
 1.0683462581800849 1.7531014184924563 33.0584697154871208 T T T
 6.3335367565219602 4.7597335717444524 32.2982219336606917 T T T
 7.7792518359221461 3.7409180048972499 34.6388985356449552 T T T
 2.0299916193227250 4.0354180359538283 34.8002652213303918 T T T
 3.1865871048511156 6.2641132396243266 33.4190021648398954 T T T
 1.9155531011895139 8.8134749983090526 32.7166404116880472 T T T
 4.7938077769610592 9.0261869856833794 32.4233010098575036 T T T
 4.9377631038286349 6.7209871240043295 32.0145648678667598 T T T

VASP input file (INCAR):

INCAR created by Atomic Simulation Environment

ENCUT = 500.000000

SIGMA = 0.050000

EDIFF = 1.00e-04

EDIFFG = -3.00e-02

PREC = Accurate

GGA = RP

ALGO = Normal

ISPIN = 1

ISMEAR = 0

NELM = 250

NEDOS = 2001

LORBIT = 11

NSW = 1000

IBRION = 2

NPAR = 1

KPAR = 7

LVHAR = .TRUE.

POTIM = 0.1

LDIPOL = .TRUE.

IDIPOL = 3

DIPOL = 0.5 0.5 0.5

VASP geometry file (POSCAR) for implicit solvent:

Pt

1.0000000000000000

8.4624236950871214 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.7715651967104353 0.0000000000000000

0.0000000000000000 0.0000000000000000 63.0317953550510666

48

Selective dynamics

Cartesian

1.4104039491811668 0.8142970997258927 30.3643076752921353 F F F

0.0000000000000000 1.6285941994517161 32.6674876797589278 F F F

2.8051035889902196 9.7669398574783273 34.9872922196833684 T T T

0.0000000000000000 3.2571883989035015 30.3643076752921353 F F F

7.0520197459059544 4.0714854986293245 32.6674876797589278 F F F

1.3926348156825556 2.4365791770095950 34.9903683897533071 T T T

4.2312118475435607 0.8142970997258927 30.3643076752921353 F F F

2.8208078983623937 1.6285941994517161 32.6674876797589278 F F F

5.6266785290954342 9.7668451578002937 34.9932829591354704 T T T

2.8208078983623937 3.2571883989035015 30.3643076752921353 F F F

1.4104039491811668 4.0714854986293245 32.6674876797589278 F F F

4.2135323017532471 2.4372260056956048 34.9886181229779680 T T T

7.0520197459059544 0.8142970997258927 30.3643076752921353 F F F

5.6416157967247278 1.6285941994517161 32.6674876797589278 F F F

8.4468550562528932 9.7678201438428491 34.9910236852268000 T T T

5.6416157967247278 3.2571883989035015 30.3643076752921353 F F F

4.2312118475435607 4.0714854986293245 32.6674876797589278 F F F

7.0362194741300561 2.4361771845001958 34.9920142733825799 T T T

1.4104039491811668 5.7000796980811108 30.3643076752921353 F F F
 0.0000000000000000 6.5143767978069338 32.6674876797589278 F F F
 2.8065296176568011 4.8780206811068876 34.9887541654504162 T T T
 0.0000000000000000 8.1429709972587201 30.3643076752921353 F F F
 7.0520197459059544 8.9572680969845422 32.6674876797589278 F F F
 1.3980757262828829 7.3224757277401347 34.9892566228537802 T T T
 4.2312118475435607 5.7000796980811108 30.3643076752921353 F F F
 2.8208078983623937 6.5143767978069338 32.6674876797589278 F F F
 5.6276514195045939 4.8780858006909993 34.9928949236482154 T T T
 2.8208078983623937 8.1429709972587201 30.3643076752921353 F F F
 1.4104039491811668 8.9572680969845422 32.6674876797589278 F F F
 4.2219888547117188 7.3225176395860432 34.9872269874543420 T T T
 7.0520197459059544 5.7000796980811108 30.3643076752921353 F F F
 5.6416157967247278 6.5143767978069338 32.6674876797589278 F F F
 8.4475314663773542 4.8778987418524995 34.9909434303033109 T T T
 5.6416157967247278 8.1429709972587201 30.3643076752921353 F F F
 4.2312118475435607 8.9572680969845422 32.6674876797589278 F F F
 7.0385443875252083 7.3223076769865356 34.9873652037738410 T T T
 2.8065373811579675 0.0110278363375612 28.0429048801058123 T T T
 1.3930056745594286 2.4525232157512695 28.0413706692065112 T T T
 5.6276908305896338 0.0111646571315617 28.0387986311240702 T T T
 4.2138311744173196 2.4518668473365874 28.0431378620680682 T T T
 8.4475517933577198 0.0113733776650661 28.0407397137379668 T T T
 7.0365769257918336 2.4530078687121484 28.0397776174425140 T T T
 2.8056350060936075 4.8936849334893804 28.0444659415480366 T T T
 1.3982373256819600 7.3382012727304637 28.0424304654950980 T T T
 5.6271938020974099 4.8939048594663515 28.0384397408463073 T T T

4.2221433228863834 7.3381017833204059 28.0444385994903129 T T T
8.4473833399928075 4.8930224498548025 28.0407539929288170 T T T
7.0386782921732856 7.3385073464399033 28.0443709805462298 T T T

VASP input file (INCAR): INCAR created by Atomic Simulation Environment

ENCUT = 500.000000

SIGMA = 0.050000

EDIFF = 1.00e-04

EDIFFG = -5.00e-02

PREC = Accurate

GGA = RP

ALGO = Normal

ISPIN = 1

ISMEAR = 0

NELM = 250

NEDOS = 2001

LORBIT = 11

NSW = 0

IBRION = 2

NPAR = 1

KPAR = 7

LVHAR = .TRUE.

LSOL = .TRUE.

LAMBDA_D_K = 3.0

TAU = 0.0

LCHARG = .FALSE.

LWAVE = .TRUE.

LVTOT = .FALSE.

NELECT = 481.111222017

LRHOB = .TRUE.

LRHOION = .TRUE.

Figure 4(a)

VASP geometry file (POSCAR) for initial (charged) state:

H O Pt

1.0000000000000000

8.5277080000000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.9234739999999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 58.5030690000000035

9 4 18

Selective dynamics

Cartesian

1.3028120619920001 2.3830943497979997 31.9575939565950051 T T T

8.1878106145360015 4.7458695223979994 31.7780480378339973 T T T

7.0961872411640003 4.5841727892900002 33.1522266255750040 T T T

3.8101117127360005 2.1505586727779997 33.2689987512990015 T T T

4.6006558274599998 2.1540395688959997 31.9116105443610003 T T T

0.7140420462560001 1.6794757569839998 33.2249459403420033 T T T

0.1986614855680000 3.7693920005039998 32.9539597247339984 T T T

5.3927349296239999 3.7716567985439995 33.2704028249549992 T T T

5.4064219009640002 0.4869315786000000 33.2704613280239982 T T T

8.1998858490640014 4.6450712391959996 32.7965279660550024 T T T

4.7201375442480007 2.1515039797859998 32.9063967296370024 T T T

1.1507886114760002 2.5096424020199999 32.9380468899660031 T T T

5.8876148802800001 4.5884562116699996 33.5692365014069978 T T T

1.2671406594280001 0.5887047096539999 27.3209332230000044 F F F

4.1097156779000006 0.5887047096539999 27.3209332230000044 F F F

6.9522821686640004 0.5887047096539999 27.3209332230000044 F F F

8.3735696779000008 3.0504417096539997 27.3209332230000044 F F F

2.6884281686640001 3.0504417096539997 27.3209332230000044 F F F
5.5309946594280008 3.0504417096539997 27.3209332230000044 F F F
8.3735696779000008 1.4092804273380000 24.9999994696320016 F F F
2.6884281686640001 1.4092804273380000 24.9999994696320016 F F F
5.5309946594280008 1.4092804273380000 24.9999994696320016 F F F
6.9522821686640004 3.8710174273379994 24.9999994696320016 F F F
1.2671406594280001 3.8710174273379994 24.9999994696320016 F F F
4.1097156779000006 3.8710174273379994 24.9999994696320016 F F F
8.3729812660480007 4.6871866357919991 29.6085202270380066 T T T
2.6892127178000003 4.6770984375659994 29.5938359567190048 T T T
5.5319327073080000 4.6805793336839994 29.5972876377900000 T T T
6.9554288929160002 2.2204818505259998 29.5936019444430052 T T T
1.2743039341480003 2.2187980224179999 29.6079351963480022 T T T
4.1137748669080008 2.2185863130360000 29.6147215523520018 T T T

VASP input file (INCAR) for initial (charged) state:

INCAR created by Atomic Simulation Environment

ENCUT = 500.000000

SIGMA = 0.050000

EDIFF = 0.0001

EDIFFG = -0.05

PREC = Accurate

GGA = PE

ALGO = Normal

ISPIN = 1

ISMEAR = 0

ICHARG = 1

NELM = 250

LVHAR = .TRUE.

NPAR = 1

KPAR = 7

IBRION = 2

POTIM = 0.1

NSW = 0

ISTART = 1

LSOL = .TRUE.

LAMBDA_D_K = 3.0

TAU = 0

NELECT = 213.24228848

LRHOB = .TRUE.

LRHOION = .TRUE.

Figure 4(b)

VASP geometry file (POSCAR) for final (uncharged) state:

H O Pt

1.0000000000000000

8.5277080000000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.9234739999999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 58.8391400000000004

9 4 18

Selective dynamics

Cartesian

1.3373236962680000 2.2330760970179999 31.2487611843199993 T T T

8.4209325681320006 4.7506255982819994 32.1037527276600017 T T T

7.4203851162000003 4.7570261144819996 33.3103669716400006 T T T

3.2269870396960005 2.2971600346019998 33.2617658420000026 T T T

4.2595219243360001 2.2993509805319996 32.0869835727599977 T T T

0.8478588401920001 1.5011032174379999 33.4741162982600002 T T T

0.8480038112280001 3.0801351813479996 33.4716450543799979 T T T

5.1467361369480003 3.9754344639299997 33.5137738786200003 T T T

5.1485951772920000 0.6267188524079998 33.5137738786200003 T T T

8.3961084101440004 4.7545446835859995 33.0910146577199953 T T T

4.2040832946280000 2.2999122565679997 33.0745985376600018 T T T

1.4058694131720002 2.2912567892759999 33.6769936529800020 T T T

5.6779952899320003 4.7621563743899991 33.7857283836999969 T T T

1.2671406594280001 0.5887047096539999 27.3209543936199992 F F F

4.1097156779000006 0.5887047096539999 27.3209543936199992 F F F

6.9522821686640004 0.5887047096539999 27.3209543936199992 F F F

8.3735696779000008 3.0504417096539997 27.3209543936199992 F F F

2.6884281686640001 3.0504417096539997 27.3209543936199992 F F F
 5.5309946594280008 3.0504417096539997 27.3209543936199992 F F F
 8.3735696779000008 1.4092804273380000 24.9999856771799998 F F F
 2.6884281686640001 1.4092804273380000 24.9999856771799998 F F F
 5.5309946594280008 1.4092804273380000 24.9999856771799998 F F F
 6.9522821686640004 3.8710174273379994 24.9999856771799998 F F F
 1.2671406594280001 3.8710174273379994 24.9999856771799998 F F F
 4.1097156779000006 3.8710174273379994 24.9999856771799998 F F F
 8.3761876842560010 4.6750699662779995 29.5857317313600028 T T T
 2.7025415254039999 4.6755327728339999 29.5698451635599966 T T T
 5.5403921936440002 4.6779354281459993 29.5972642028000017 T T T
 6.9594624988000007 2.2176065417099999 29.5852021791000013 T T T
 1.2791306168759999 2.2180348839480000 29.6938780706800038 T T T
 4.1210831126640004 2.2176410060279999 29.5989116987200021 T T T

VASP input file for the final (uncharged) state:
INCAR created by Atomic Simulation Environment
ENCUT = 500.000000
SIGMA = 0.050000
EDIFF = 0.0001
EDIFFG = -0.05
PREC = Accurate
GGA = PE
ALGO = Normal
ISPIN = 1
ISMEAR = 0
ICHARG = 1
NELM = 250
LVHAR = .TRUE.
NPAR = 1
KPAR = 7
IBRION = 2
POTIM = 0.1
NSW = 0
ISTART = 1
LSOL = .TRUE.
LAMBDA_D_K = 3.0
TAU = 0
NELECT = 213.757600104
LRHOION = .TRUE.

Figure 5(a)

Table corresponding to data in Figure 5(a):

U / V vs SHE	$\Delta\Omega_{\text{CO}_2, \varepsilon_{\text{b}}} = 1.0$	$\Delta\Omega_{\text{CO}_2, \varepsilon_{\text{b}}} = 4.0$	$\Delta\Omega_{\text{CO}_2, \varepsilon_{\text{b}}} = 78.4$
0.65	0.631001	0.511753	0.359526
0.9	0.652091	0.538041	0.407218
1.05	0.661741	0.55973	0.432668
1.15	0.670024	0.581508	0.452283
1.25	0.676996	0.587738	0.482089
1.4	0.687004	0.614703	0.533251
1.65	0.708277	0.655352	0.559279

Figure 5(b)

Table corresponding to data in Figure 5(b):

U / V vs SHE	$\Delta\Omega_{\text{H}, \varepsilon_{\text{b}}} = 1.0$	$\Delta\Omega_{\text{H}, \varepsilon_{\text{b}}} = 4.0$	$\Delta\Omega_{\text{H}, \varepsilon_{\text{b}}} = 78.4$
-1.25	-0.158573	-0.417679	-0.844913
-1.00	-0.067192	-0.375467	-0.765804
-0.5	-0.021835	-0.251868	-0.513187
0.0	0.042722	-0.085753	-0.124068
0.5	0.123274	0.096372	0.141222

The point for explicit charge extrapolation is at (-0.615, -0.14004853) with slope 0.5067.

References

- (1) Bockris, *Modern Electrochemistry 2A*; Kluwer Academic Publishers: Boston, 2002; Vol. 86; pp 911–916.
- (2) Trasatti, S.; Lust, E. *Modern Aspects of Electrochemistry*; Springer, 2002; pp 1–215.