Electronic Supplementary Information (ESI)

Shear adhesive strength between epoxy resin and copper surfaces: a density functional theory study

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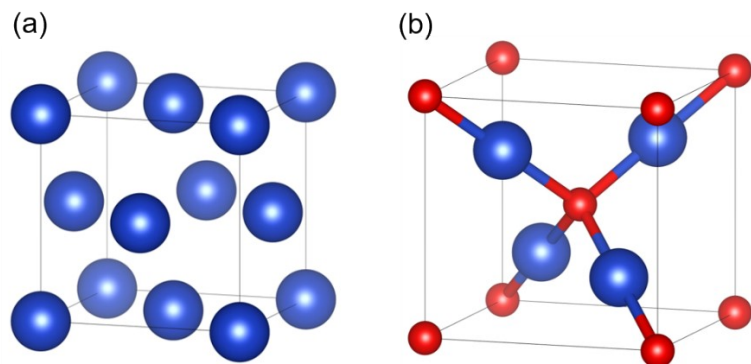*Corresponding author Email: kazunari@ms.ifoc.kyushu-u.ac.jp

Fig. S1 (a) Optimized Cu unit cell. (b) Optimized Cu_2O unit cell. The blue and red atoms correspond to copper and oxygen atoms, respectively.
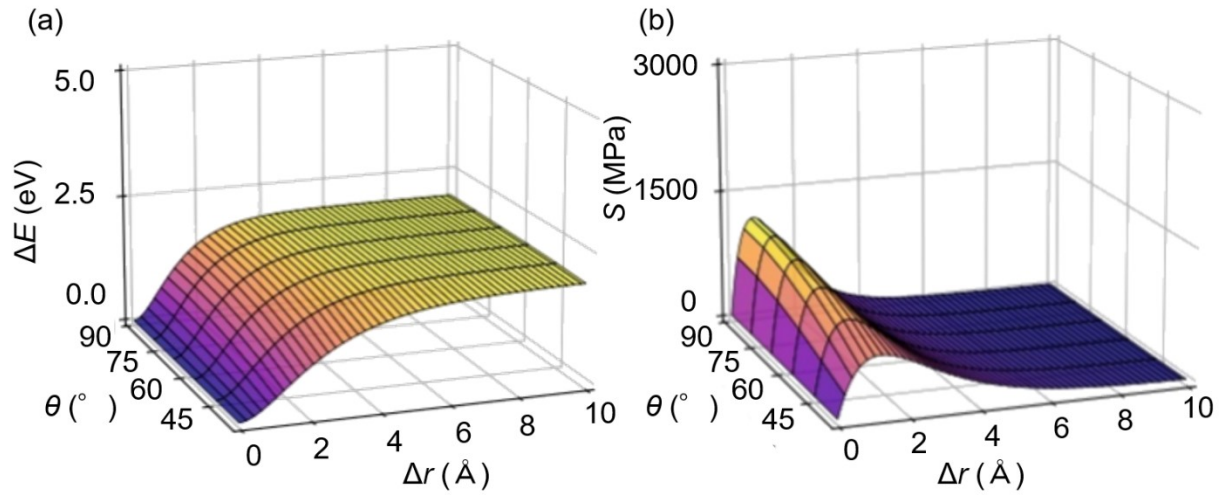
Fig. S2 (a) and (b) show 3D plot of the energy and adhesive stress surfaces of the epoxy molecule on the Cu(111) surface.
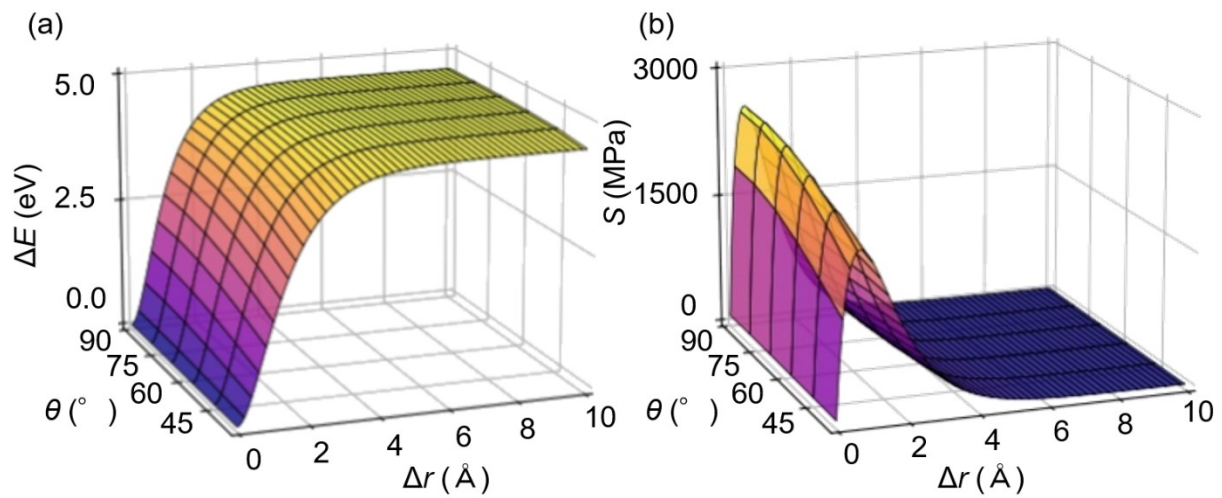

Fig. S3 (a) and (b) show 3D plot of the energy and adhesive stress surfaces of the epoxy molecule on the $Cu_2O(111)$ surface.

Fig. S4 Plots of the computed values in the range of $33.75° \leq \theta \leq 90.00°$ for the epoxy molecule/Cu(111) surface. Each point in the dotted line corresponds to the value obtained by the single-point calculation, and the curves obtained by fitting them are represented as the black, blue, and red solid lines: Black corresponds to total, blue to dispersion, and red to DFT.

Fig. S5 Plots of the computed values in the range of $0.0000° \leq \theta \leq 33.7500°$ for the epoxy molecule/Cu(111) surface. Each point in the dotted line corresponds to the value obtained by the single-point calculation, and the curves obtained by fitting them are represented as the black, blue, and red solid lines: Black corresponds to total, blue to dispersion, and red to DFT.
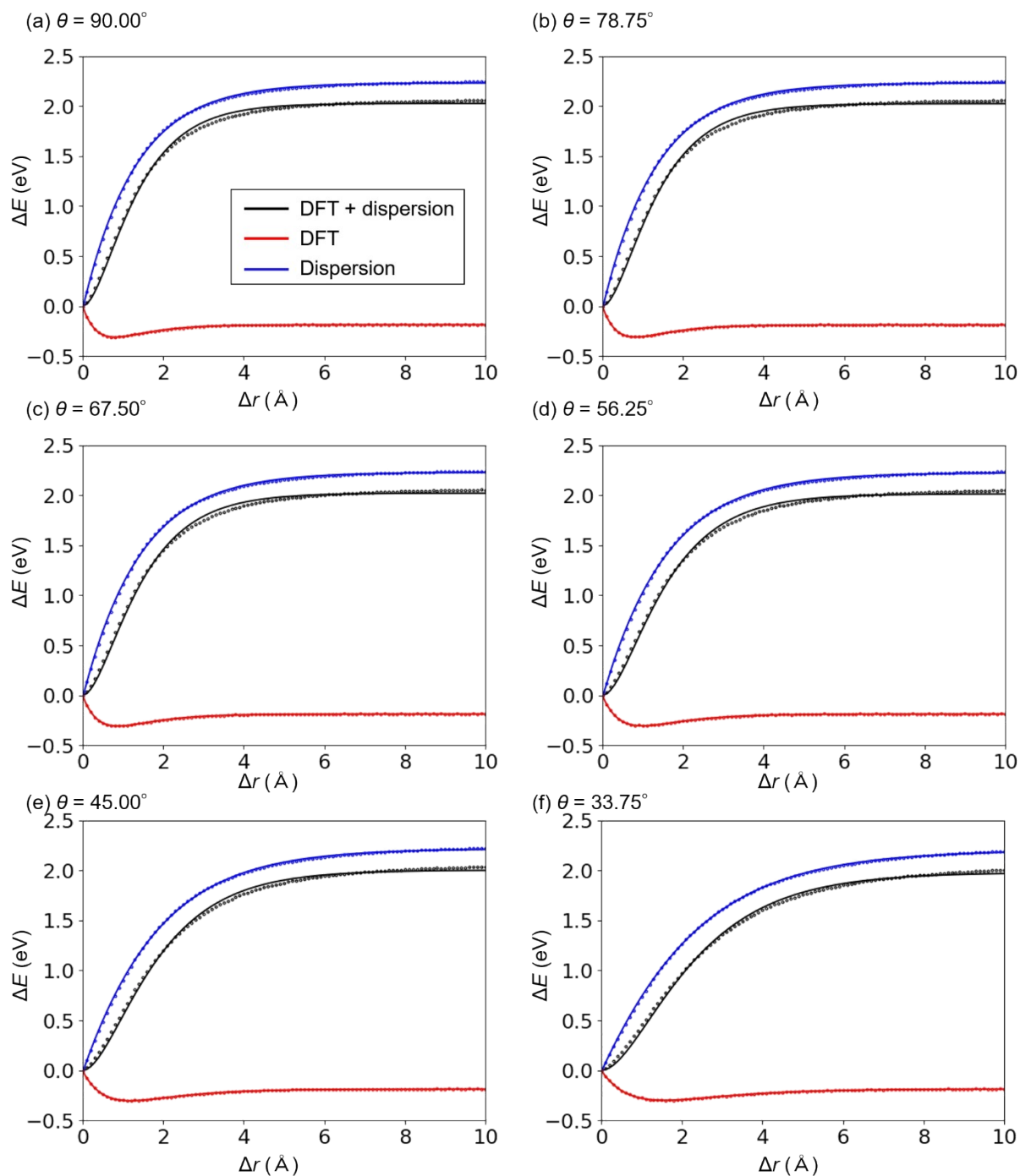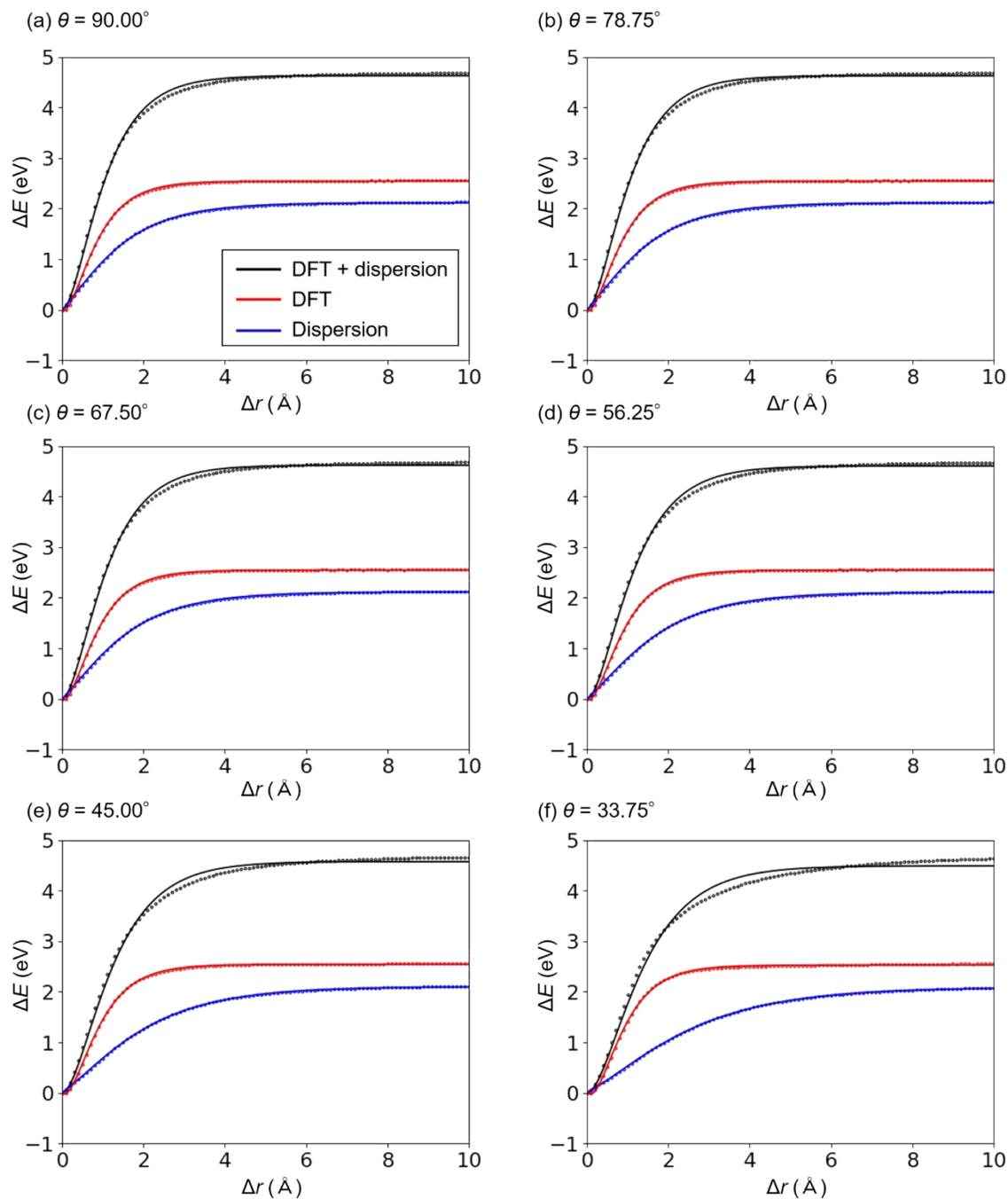
Fig. S6 Plots of the computed values in the range of $33.75° \leq \theta \leq 90.00°$ for the epoxy molecule/$Cu_2O(111)$ surface. Each point in the dotted line corresponds to the value obtained by the single-point calculation, and the curves obtained by fitting them are represented as the black, blue, and red solid lines: Black corresponds to total, blue to dispersion, and red to DFT.
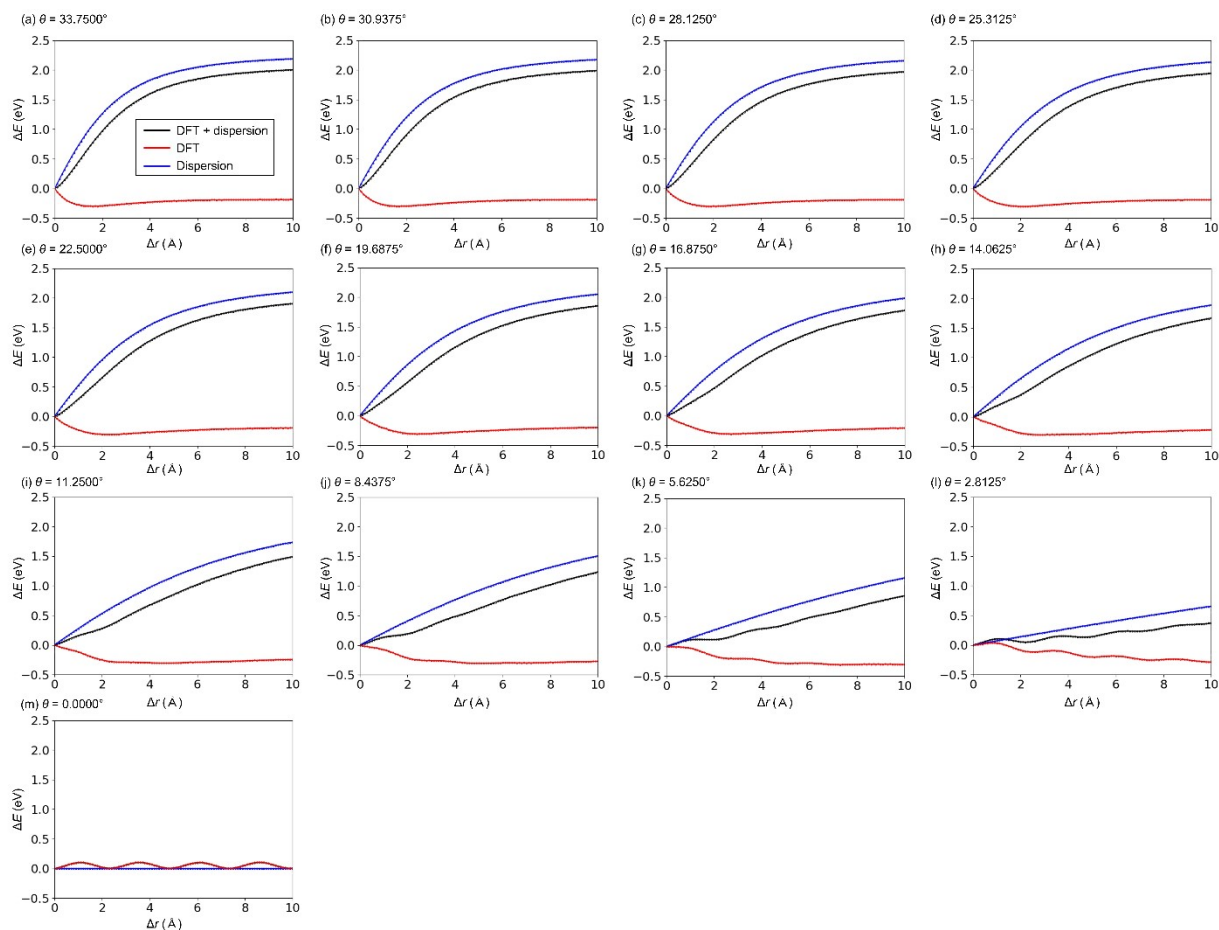
Fig. S7 Plots of the computed values in the range of $0.0000° \leq \theta \leq 33.7500°$ for the epoxy molecule/Cu_2O(111) surface. Each point in the dotted line corresponds to the value obtained by the single-point calculation, and the curves obtained by fitting them are represented as the black, blue, and red solid lines: Black corresponds to total, blue to dispersion, and red to DFT.

(a) Side-view	(b) Side-view
Top-view	Top-view

Total DFT energy	-491.012 eV	-714.854 eV
	-4.632 eV/atom	-5.034 eV/atom
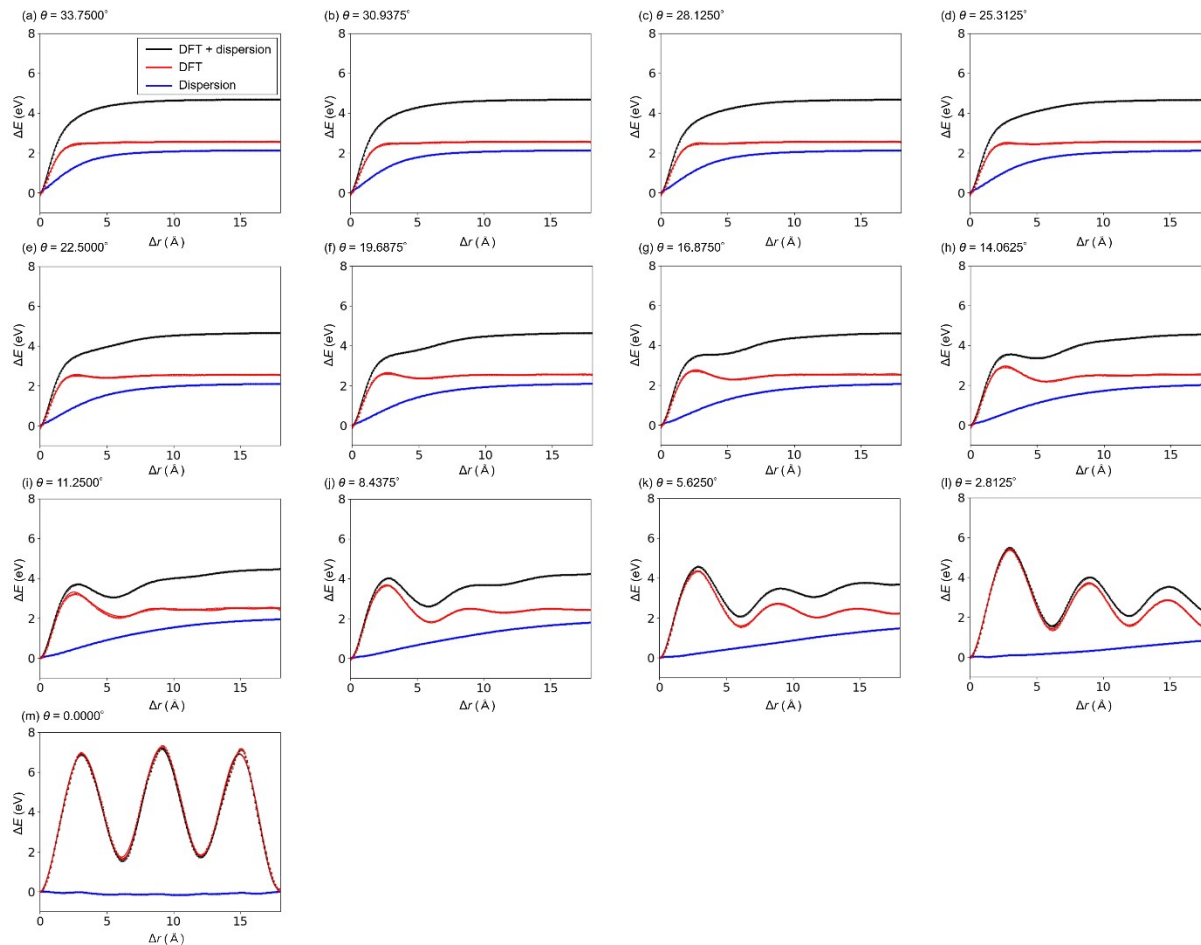
Fig. S8 Total DFT energy of (a) the epoxy/Cu(111) surface and (b) the epoxy/Cu$_2$O(111) surface, which was calculated in the way that the atomic reference energies were subtracted from the whole DFT energy of the unit cell, so that it can be regarded as an approximate cohesive energy or the atomization energy of the compound of a certain kind.

The OH groups of the epoxy resin interacted with (a) the Cu(111) surface, and the two benzene rings of the epoxy resin interacted with the OH groups for (b)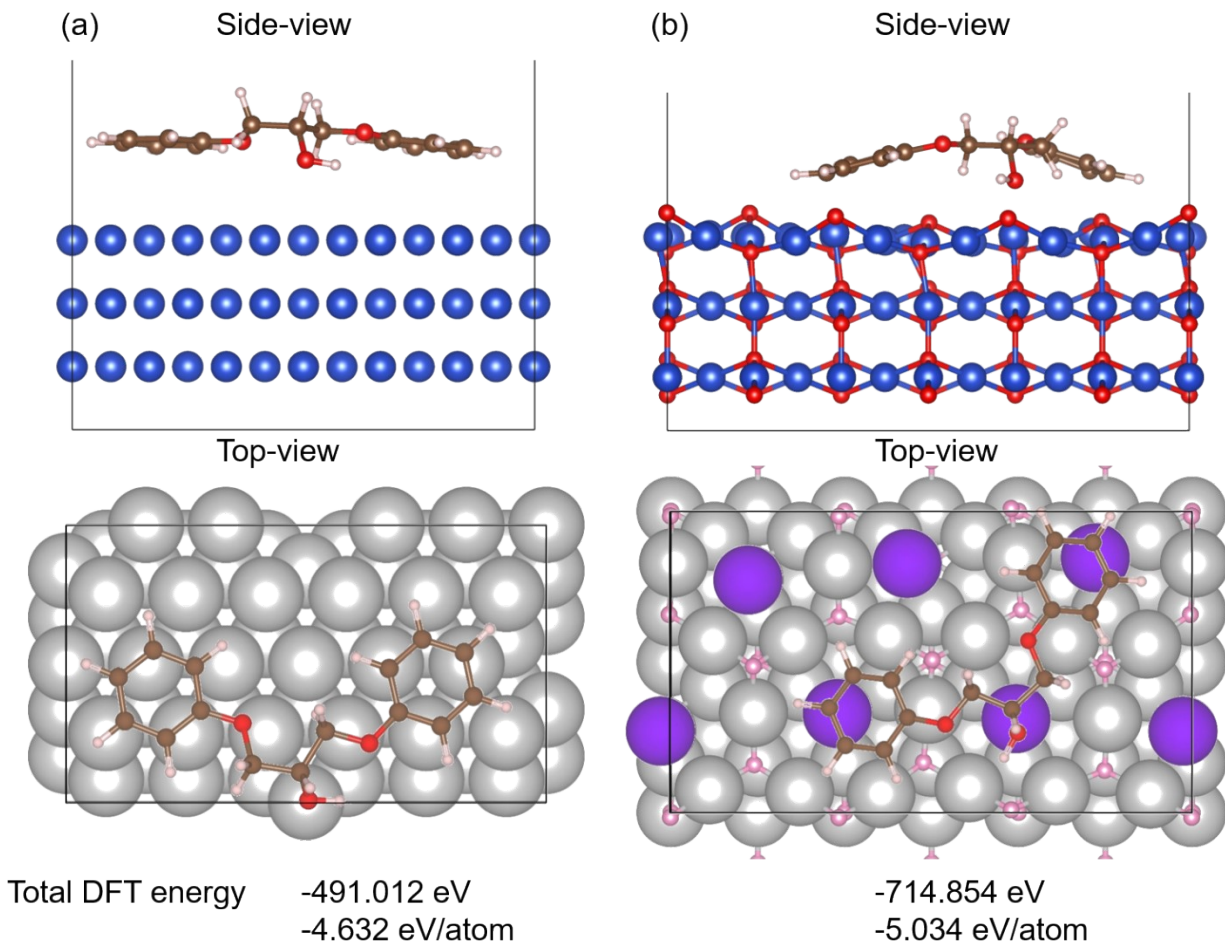 the $Cu_2O(111)$ surface. Molecular interactions are visualized by isosurfaces of charge density difference in Fig. S9.

The crystal orbital Hamilton population (COHP) analysis[1] was performed to estimate the strength of the interactions using LOBSTER[2]. The values in the projected COHP (pCOHP) plots shown in Fig. S9 have been multiplied by -1 so that positive -pCOHP values means binding interactions. The dashed line indicates the Fermi level. The positive -pCOHP values below the Fermi level in (b) are larger than in (a). In both (a) and (b), the bonding type orbital interactions exist over a relatively wide energy range. To compare the orbital interaction energies, the pCOHP values were integrated up to the Fermi level for each atomic pair. These are called ICOHP. A negative ICOHP value can be read as bonding energy. Comparison of the ICOHPs shows that all of the interactions in (b) are larger than in (a).

References:

1. R. Dronskowski and P. E. Bloechl, *J. Phys. Chem*., 1993, **97**, 8617-8624.

2. V. L. Deringer, A. L. Tchougreeff and R. Dronskowski, *J. Phys. Chem. A,* 2011, **115**, 5461-5466.
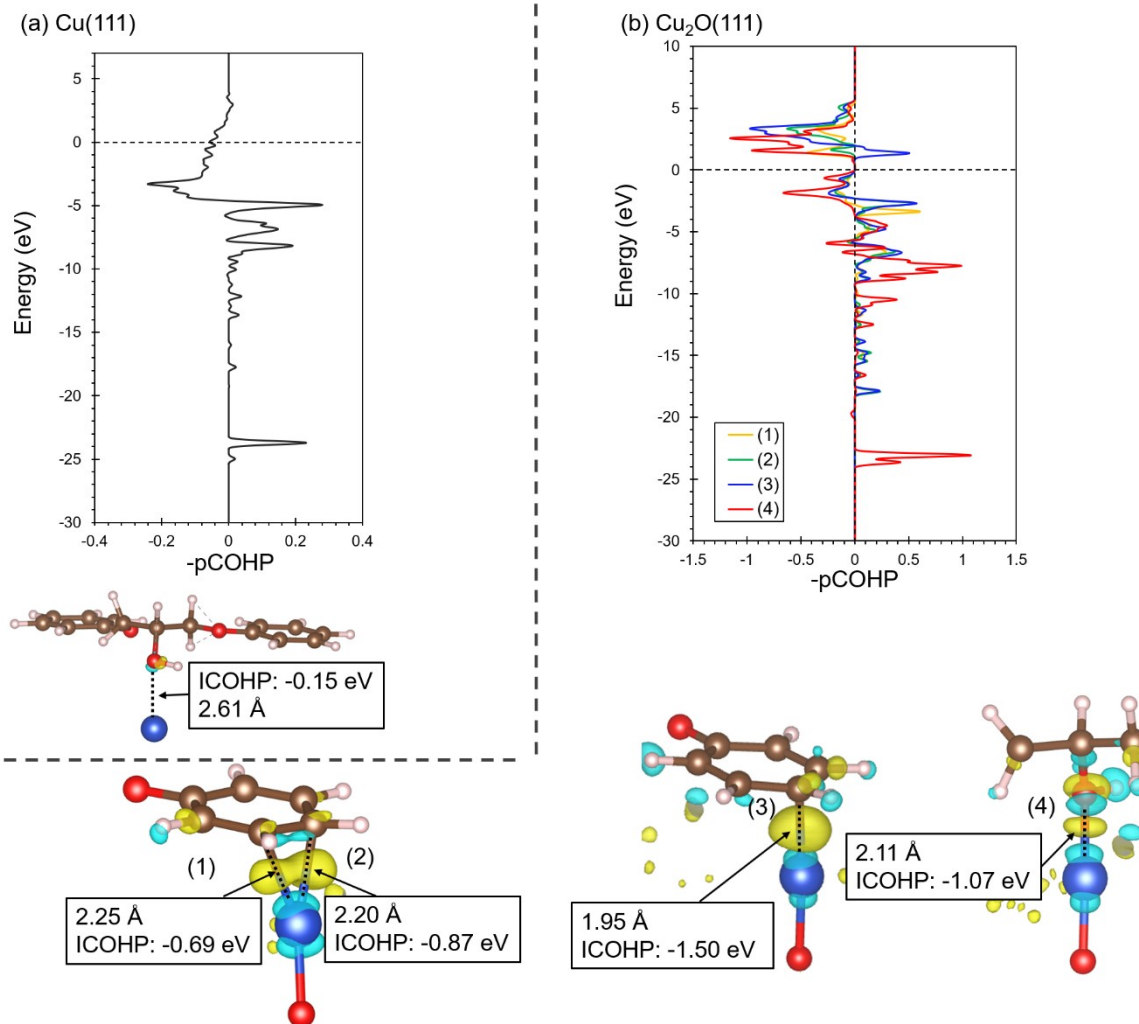
Fig. S9 Negative of pCOHP (-pCOHP), atomic distances (Å) and integrated pCOHP (ICOHP) for interactions between the epoxy resin and the surfaces. (a) The interaction between the OH group and the Cu(111) surface. (b) The interaction of (1), (2), and (3) the benzene ring, (4) the OH group for the Cu$_2$O(111). Molecular interactions are visualized by isosurfaces of charge density difference. Yellow and cyan indicate charge accumulation and depletion, respectively. The isovalue is set to 0.005.

$$E = D(1 - \exp(-a(\Delta r - \alpha)))^2 + \sum_{i=1}^{5} b_i \cos(c_i \Delta r - d_i) + \beta \quad \#(S1)$$

Table S1. Values of the fitting parameters using eqn (S1) for the energy curves of the epoxy molecule for Cu(111) surface. Eqn (S1) is the same as eqn (4) in the main text.

θ (°)	0.0000	2.8125	5.6250	8.4375	11.2500	14.0625	16.8750	19.6875	22.5000	25.3125	28.1250	30.9375	33.7500
D (eV)	0.00	4.31	1.32	2.12	1.61	1.76	2.05	2.80	2.78	1.64	2.32	1.00	1.24
a (Å^{-1})	2.70	0.03	0.15	0.14	0.28	0.29	0.53	0.84	0.91	1.11	0.88	1.38	1.01
b_1 (eV)	-0.20	-1.07	0.01	12.18	-0.06	-0.66	0.35	-5.29	-1.76	-1.11	-0.72	-0.86	-0.61
b_2 (eV)	-1.21	0.06	0.45	-11.3	1.16	1.66	0.29	-1.70	-0.66	-0.01	-0.24	-0.33	0.02
b_3 (eV)	0.76	0.03	0.45	8.88	1.11	-1.52	0.17	-4.22	0.00	1.01	0.17	0.23	0.26
b_4 (eV)	0.77	-1.00	0.00	-4.75	-0.49	0.73	-0.05	-1.95	-0.05	-0.29	-0.19	0.02	-0.05
b_5 (eV)	0.05	1.99	0.02	3.26	0.44	0.08	1.08	-1.09	1.03	0.79	0.78	1.06	0.61
c_1 (Å^{-1})	0.94	1.80	1.75	1.98	0.53	1.71	1.56	1.06	0.24	0.81	0.92	0.81	0.41
c_2 (Å^{-1})	0.63	1.31	2.38	2.08	2.31	1.99	1.72	1.30	0.94	1.61	1.71	1.38	1.68
c_3 (Å^{-1})	0.79	2.49	2.39	1.88	2.21	1.86	1.20	1.22	2.20	0.92	1.75	1.54	0.97
c_4 (Å^{-1})	0.48	1.66	3.67	2.13	2.37	2.07	1.97	0.95	1.39	1.12	1.38	1.87	1.51
c_5 (Å^{-1})	2.49	1.74	7.38	1.81	2.12	1.32	0.17	0.93	0.77	0.62	0.76	0.63	0.70
d_1	1.62	3.35	3.14	4.04	2.48	7.63	1.24	2.34	1.31	1.68	1.15	0.00	1.52
d_2	0.02	6.97	3.83	-1.74	0.76	0.00	-0.88	-2.36	0.00	-0.99	0.01	0.59	-5.21
d_3	0.85	8.42	0.79	6.65	3.23	5.45	2.07	0.23	8.36	3.05	0.38	1.58	-3.67
d_4	-0.73	2.57	8.18	-4.59	1.18	-2.67	-5.57	-1.46	-0.13	-1.35	1.06	0.41	0.00
d_5	8.93	3.01	1.00	9.45	5.82	5.24	3.97	-1.96	-1.13	-0.59	0.00	-1.28	-2.44
α (Å)	2.86	0.01	0.03	-0.55	0.00	0.33	0.00	-0.44	-0.62	-0.50	-0.46	-0.41	-0.38
β (eV)	0.17	0.07	0.03	0.03	0.00	0.10	0.55	-1.23	0.20	-0.01	-0.58	0.62	0.64

Table S2. Values of the fitting parameters using eqn (S1) for the energy curves of the epoxy molecule for $Cu_2O(111)$ surface. Eqn (S1) is the same as eqn (4) in the main text.

θ (°)	0.0000	2.8125	5.6250	8.4375	11.2500	14.0625	16.8750	19.6875	22.5000	25.3125	28.1250	30.9375	33.7500
D (eV)	1.63	-0.34	2.97	4.08	2.46	5.79	5.90	6.17	6.34	6.45	6.46	6.41	6.25
a (Å^{-1})	1.91	7.21	0.83	0.59	0.13	0.15	0.72	0.78	0.83	0.89	0.95	1.00	1.06
b_1 (eV)	23.90	0.04	-8.01	-18.4	-533.7	-746.9	136.6	-5.29	-1.76	-1.11	-90.79	92.46	33.05
b_2 (eV)	44.14	1.82	-0.40	37.17	-558.0	-298.9	-50.63	-1.70	-0.66	-0.01	84.92	107.5	-29.22
b_3 (eV)	0.08	0.19	0.04	19.09	-220.7	-286.8	120.5	-4.22	0.00	1.01	-37.24	-86.37	12.47
b_4 (eV)	-0.40	-27.5	-0.02	-5.13	-666.4	-926.7	108.5	-1.95	-0.05	-0.29	-32.98	-37.84	10.65
b_5 (eV)	-41.7	-26.6	-7.96	-5.14	-204.6	-765.5	-41.88	-1.09	1.03	0.79	-105.6	33.55	-26.89
c_1 (Å^{-1})	0.02	2.20	0.69	0.80	1.42	1.44	-1.00	1.06	0.24	0.81	0.92	0.91	0.96
c_2 (Å^{-1})	0.99	0.96	1.13	0.76	1.33	1.34	0.88	1.30	0.94	1.61	1.04	0.97	0.87
c_3 (Å^{-1})	1.94	1.32	1.57	0.72	1.30	1.46	0.93	1.21	2.20	0.92	0.87	1.03	0.82
c_4 (Å^{-1})	0.61	0.70	2.29	1.84	1.37	1.40	1.06	0.95	1.39	1.11	1.08	0.87	1.07
c_5 (Å^{-1})	0.98	0.70	0.67	1.84	1.44	1.36	1.09	0.93	0.77	0.62	0.98	1.06	1.03
d_1	-6.19	10.93	3.39	-4.29	-3.29	-3.15	0.13	2.34	1.31	1.68	5.13	1.81	5.45
d_2	2.82	2.12	6.28	-4.75	2.04	5.16	1.98	-2.36	0.00	-0.99	-2.89	-0.63	4.52
d_3	10.79	4.65	5.63	-2.09	4.88	-6.04	2.49	0.23	8.36	3.04	1.51	0.03	3.93
d_4	-9.45	-1.06	8.36	3.11	-0.61	-0.43	-2.31	-.146	-0.13	-1.35	-2.50	1.36	0.47
d_5	-3.51	2.00	0.00	-0.04	-6.15	2.29	-1.91	-1.96	-1.13	-0.59	2.72	0.40	0.00
α (Å)	-0.01	0.00	0.31	0.67	-0.84	-8.35	0.36	0.26	0.18	0.11	0.05	0.01	-0.01
β (eV)	-11.5	1.20	-1.95	0.00	2.32	-1.69	-1.50	-0.96	-1.57	-2.14	0.41	0.32	-11.34

$$E = \sum_{i=0}^{12} e_i (\Delta r)^i \quad \#(S2)$$

Table S3 Values of the fitting parameters using eqn (S2) for the energy curves of the epoxy molecule for Cu(111) surface. Eqn (S2) is the same as eqn (7) in the main text.

θ (°)	0.0000	2.8125	5.6250	8.4375	11.2500	14.0625	16.8750	19.6875	22.5000	25.3125	28.1250	30.9375	33.7500
e_0 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_1 (eV/Å)	0.00	0.07	0.14	0.21	0.28	0.35	0.42	0.49	0.56	0.63	0.69	0.75	0.81
e_2 (eV/Å)	-0.01	-0.01	0.00	0.00	0.01	-0.01	-0.02	-0.02	-0.03	-0.04	-0.05	-0.06	-0.07
e_3 (eV/Å)	0.02	0.01	0.01	0.00	0.00	0.00	-0.01	-0.01	-0.01	0.01	-0.01	-0.01	-0.01
e_4 (eV/Å)	-0.02	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_5 (eV/Å)	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_6 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_7 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_8 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_9 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_{10} (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_{11} (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_{12} (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4 Values of the fitting parameters using eqn (S2) for the energy curves of the epoxy molecule for $Cu_2O(111)$ surface. Eqn (S2) is the same as eqn (7) in the main text.

θ (°)	0.0000	2.8125	5.6250	8.4375	11.2500	14.0625	16.8750	19.6875	22.5000	25.3125	28.1250	30.9375	33.7500
e_0 (eV/Å)	-0.02	-0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01
e_1 (eV/Å)	0.30	0.22	0.20	0.21	0.24	0.26	0.28	0.31	0.33	0.36	0.39	0.42	0.45
e_2 (eV/Å)	-0.81	-0.49	-0.31	-0.24	-0.20	-0.15	-0.11	-0.06	-0.02	0.01	0.05	0.08	0.11
e_3 (eV/Å)	0.77	0.45	0.28	0.21	0.18	0.15	0.12	0.09	0.06	0.03	0.01	-0.02	-0.04
e_4 (eV/Å)	-0.38	-0.21	-0.13	-0.10	-0.08	-0.07	-0.06	-0.05	-0.04	-0.03	-0.02	-0.01	0.00
e_5 (eV/Å)	0.11	0.06	0.04	0.03	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.00
e_6 (eV/Å)	-0.02	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_7 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_8 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_9 (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_{10} (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_{11} (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
e_{12} (eV/Å)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

$$E = \sum_{i=1}^{5} b_i \cos\left(c_i \Delta r - d_i\right) + \beta \ \#(S3)$$

Table S5 Values of the fitting parameters using eqn (S3) for the energy curves of the epoxy molecule for Cu(111) surface. Eqn (S3) is the same as eqn (8) in the main text.

θ (°)	0.0000	2.8125	5.6250	8.4375	11.2500	14.0625	16.8750	19.6875	22.5000	25.3125	28.1250	30.9375	33.7500
b_1 (eV)	-0.05	0.07	-0.04	-0.35	-2.08	-1382	-1956	-1508	213.58	241.09	43.66	68.26	-118.2
b_2 (eV)	-1.08	-0.01	-0.01	-4.14	-0.04	-328.5	-2208	-1617	616.47	1308.1	182.24	405.07	353.65
b_3 (eV)	-0.16	0.90	-1.00	-8.28	104.61	1632.8	2377.7	-323.0	-1130	-1188	-122.9	-311.4	-700.0
b_4 (eV)	0.86	-5.66	4.30	-4.14	2.12	949.72	482.27	1328.9	910.82	-693.7	-236.9	-204.3	533.68
b_5 (eV)	1.39	-0.89	0.99	5.01	37.48	1541.4	1354.4	912.72	1044.8	-1028	-214.4	-364.5	623.23
c_1 (Å^{-1})	2.49	0.27	0.46	0.32	2.46	0.58	0.54	0.39	0.72	0.69	0.81	0.76	0.71
c_2 (Å^{-1})	0.35	2.06	2.66	2.49	2.24	0.76	0.39	0.20	0.66	0.19	0.61	0.21	0.65
c_3 (Å^{-1})	0.91	2.47	2.10	2.48	0.07	0.21	0.20	0.71	0.20	0.37	0.74	0.57	0.20
c_4 (Å^{-1})	0.72	0.01	0.05	2.46	2.45	0.69	0.70	0.54	0.55	0.63	0.22	0.69	0.54
c_5 (Å^{-1})	0.57	2.48	2.09	0.09	0.12	0.41	0.65	0.65	0.39	0.52	0.44	0.41	0.39
d_1	5.78	-1.91	1.02	-0.85	2.86	-3.35	-3.53	-1.15	0.55	-5.87	-5.22	-5.42	-8.71
d_2	1.77	6.41	5.60	2.63	1.40	-2.43	-7.45	-5.27	-2.90	-2.16	0.06	-2.03	-9.04
d_3	1.52	3.87	4.36	5.67	-2.66	-2.07	4.14	3.63	7.31	-1.19	-5.57	-3.23	-5.21
d_4	0.54	-5.58	-2.71	8.72	2.83	-2.76	-5.82	-6.66	-12.90	-6.16	-5.12	-5.76	-6.48
d_5	2.88	3.92	10.62	-2.53	-5.48	-4.18	-2.98	3.33	-4.27	-3.57	-0.85	-0.94	-4.17
β (eV)	0.44	4.38	3.95	4.36	66.86	852.29	1253.4	848.84	593.41	695.01	125.28	215.73	374.81

Table S6 Values of the fitting parameters using eqn (S3) for the energy curves of the epoxy molecule for $Cu_2O(111)$ surface. Eqn (S3) is the same as eqn (8) in the main text.

θ (°)	0.0000	2.8125	5.6250	8.4375	11.2500	14.0625	16.8750	19.6875	22.5000	25.3125	28.1250	30.9375	33.7500
b_1 (eV)	4.36	0.06	-0.36	0.96	2124.4	1753.8	-1694	985.38	354.62	165.01	4906.0	4318.8	1595.8
b_2 (eV)	32.10	260.8	9387	0.54	0.15	682.74	-1621	-366.7	139.71	66.04	1887.4	-4274	-5125
b_3 (eV)	1.69	506.8	40183	134.5	5073.4	-2108	-4393	-386.1	-423.7	-159.5	-6019	1659.1	4167.6
b_4 (eV)	-20.0	95.15	-25789	139.8	5004.6	-636.9	-4274	-954.9	-133.6	-63.23	-1863	-5291	-4150
b_5 (eV)	-16.9	246.6	35095	-274	2055.5	-1674	-5351	-1188	-342.3	-195.4	-4863	-1643	1598.0
c_1 (Å^{-1})	0.37	1.55	1.15	0.97	1.38	0.93	0.93	0.91	0.91	0.91	0.87	0.86	0.87
c_2 (Å^{-1})	0.68	0.92	0.28	0.79	0.75	0.95	0.83	0.80	0.94	0.95	0.89	0.80	0.83
c_3 (Å^{-1})	1.11	0.91	0.10	1.42	1.39	0.89	0.91	0.94	0.86	0.78	0.84	0.88	0.85
c_4 (Å^{-1})	0.75	0.00	0.25	1.40	1.40	0.83	0.85	0.83	0.77	0.74	0.80	0.83	0.80
c_5 (Å^{-1})	0.56	0.91	0.18	1.41	1.41	0.86	0.88	0.87	0.80	0.85	0.81	0.79	0.78
d_1	0.00	7.16	6.34	3.05	7.19	0.29	-6.07	0.02	0.00	0.00	-0.47	-0.56	-3.60
d_2	2.78	0.64	-3.61	3.97	3.26	-2.63	5.56	5.17	-2.82	-2.76	-3.45	1.99	-0.92
d_3	-2.35	3.66	-2.23	-1.29	4.15	-0.06	-3.10	-6.02	-0.54	1.79	-0.76	-3.53	-0.63
d_4	-2.90	-0.18	-3.93	4.80	1.15	5.63	2.60	2.30	4.81	4.48	5.05	-0.85	1.92
d_5	-4.58	6.69	1.76	-1.39	-1.89	2.72	-0.25	-0.40	2.03	-0.65	2.10	4.95	1.73
β (eV)	5.05	-90.3	21492	2.36	2.40	2.41	2.42	2.43	2.43	2.43	2.43	2.43	2.43

Table S7 The sensitivity of the energy to the number of layers to be fixed for Cu(111) surface. The surface model was fixed from the lowest layer. The model with two fixed layers is used in the main text, and the relative energy for the other models is shown.

Number of fixed layers	Energy (eV)
0	-0.02
1	-0.03
2	0.00
3	0.01

The following structural data for the epoxy resin on Cu(111) surface is provided in the VASP

POSCAR format.

Epoxy resin on Cu(111) surface
```
   1.00000000000000
    15.1403999328999994    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.7412996292000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0000000000000000
   Cu   C   H   O
    72   15   16    3
Selective dynamics
Direct
  0.0000000000000000 0.1666699949999995 0.0588700745812574  F  F  F
  0.1666699949999995 0.1666699949999995 0.0588700745812574  F  F  F
  0.3333300050000005 0.1666699949999995 0.0588700745812574  F  F  F
  0.5000000000000000 0.1666699949999995 0.0588700745812574  F  F  F
  0.6666700239999983 0.1666699949999995 0.0588700745812574  F  F  F
  0.8333299760000017 0.1666699949999995 0.0588700745812574  F  F  F
  0.0833299980000035 0.4166699949999995 0.0588700745812574  F  F  F
  0.2500000000000000 0.4166699949999995 0.0588700745812574  F  F  F
  0.4166699949999995 0.4166699949999995 0.0588700745812574  F  F  F
  0.5833299760000017 0.4166699949999995 0.0588700745812574  F  F  F
  0.7500000000000000 0.4166699949999995 0.0588700745812574  F  F  F
  0.9166700239999983 0.4166699949999995 0.0588700745812574  F  F  F
  0.0000000000000000 0.6666700239999983 0.0588700745812574  F  F  F
  0.1666699949999995 0.6666700239999983 0.0588700745812574  F  F  F
  0.3333300050000005 0.6666700239999983 0.0588700745812574  F  F  F
  0.5000000000000000 0.6666700239999983 0.0588700745812574  F  F  F
  0.6666700239999983 0.6666700239999983 0.0588700745812574  F  F  F
  0.8333299760000017 0.6666700239999983 0.0588700745812574  F  F  F
  0.0833299980000035 0.9166700239999983 0.0588700745812574  F  F  F
  0.2500000000000000 0.9166700239999983 0.0588700745812574  F  F  F
```

0.4166699949999995	0.9166700239999983	0.0588700745812574	F	F	F
0.5833299760000017	0.9166700239999983	0.0588700745812574	F	F	F
0.7500000000000000	0.9166700239999983	0.0588700745812574	F	F	F
0.9166700239999983	0.9166700239999983	0.0588700745812574	F	F	F
0.0833299980000035	0.0833299980000035	0.1177326688479852	F	F	F
0.2500000000000000	0.0833299980000035	0.1177326688479852	F	F	F
0.4166699949999995	0.0833299980000035	0.1177326688479852	F	F	F
0.5833299760000017	0.0833299980000035	0.1177326688479852	F	F	F
0.7500000000000000	0.0833299980000035	0.1177326688479852	F	F	F
0.9166700239999983	0.0833299980000035	0.1177326688479852	F	F	F
0.0000000000000000	0.3333300050000005	0.1177326688479852	F	F	F
0.1666699949999995	0.3333300050000005	0.1177326688479852	F	F	F
0.3333300050000005	0.3333300050000005	0.1177326688479852	F	F	F
0.5000000000000000	0.3333300050000005	0.1177326688479852	F	F	F
0.6666700239999983	0.3333300050000005	0.1177326688479852	F	F	F
0.8333299760000017	0.3333300050000005	0.1177326688479852	F	F	F
0.0833299980000035	0.5833299760000017	0.1177326688479852	F	F	F
0.2500000000000000	0.5833299760000017	0.1177326688479852	F	F	F
0.4166699949999995	0.5833299760000017	0.1177326688479852	F	F	F
0.5833299760000017	0.5833299760000017	0.1177326688479852	F	F	F
0.7500000000000000	0.5833299760000017	0.1177326688479852	F	F	F
0.9166700239999983	0.5833299760000017	0.1177326688479852	F	F	F
0.0000000000000000	0.8333299760000017	0.1177326688479852	F	F	F
0.1666699949999995	0.8333299760000017	0.1177326688479852	F	F	F
0.3333300050000005	0.8333299760000017	0.1177326688479852	F	F	F
0.5000000000000000	0.8333299760000017	0.1177326688479852	F	F	F
0.6666700239999983	0.8333299760000017	0.1177326688479852	F	F	F
0.8333299760000017	0.8333299760000017	0.1177326688479852	F	F	F
0.9998543171080175	0.9992604582479259	0.1775395453563490	T	T	T
0.1664263366559771	0.9989508708638889	0.1773103166775926	T	T	T
0.3325290241092181	0.9989640996638554	0.1771219419518852	T	T	T
0.4992316065819011	0.0005092538953073	0.1775953375230706	T	T	T
0.6669691617579124	-0.0008232997038633	0.1771563292744323	T	T	T

```
0.8333534876868874 -0.0008309176047076 0.1772180398806905  T  T  T
0.0831155739572244  0.2488448798352378 0.1772430036964522  T  T  T
0.2499127882311596  0.2484430646989559 0.1769782893541069  T  T  T
0.4164166275717809  0.2500991881349108 0.1770209089491300  T  T  T
0.5833618243922796  0.2497811805944748 0.1766479173043274  T  T  T
0.7498356979170959  0.2487976585125453 0.1771727681033635  T  T  T
0.9168594640594117  0.2488322424810865 0.1769270809675466  T  T  T
0.0001754637714975  0.4994340986884067 0.1769015207787104  T  T  T
0.1664867452458573  0.4999382888861762 0.1770573978811819  T  T  T
0.3331788942596611  0.4995025925980841 0.1770388872712393  T  T  T
0.4997596172125189  0.4995815298769944 0.1770722517991988  T  T  T
0.6660613144132219  0.4997725136976437 0.1771593844899304  T  T  T
0.8336394218221679  0.5001985795334094 0.1771720346613351  T  T  T
0.0831253841739748  0.7499207209653598 0.1770953811800561  T  T  T
0.2498786992172447  0.7500367936504363 0.1770860022149526  T  T  T
0.4162781623987087  0.7488963346460910 0.1770850135422608  T  T  T
0.5833944795583212  0.7497072601435960 0.1770971273523441  T  T  T
0.7497782069023567  0.7503213262401667 0.1769822149419246  T  T  T
0.9167879076727973  0.7501426371193861 0.1770588271362496  T  T  T
0.1824080297683199  0.5513110768128999 0.2654121920082016  T  T  T
0.2680044712888214  0.4925665783743062 0.2657752684382202  T  T  T
0.2813912805774146  0.3342590001814405 0.2694353085999743  T  T  T
0.2088610101817483  0.2350528777515710 0.2719913575077169  T  T  T
0.1233557790389994  0.2959898941500458 0.2714898822631875  T  T  T
0.1095317616803339  0.4534482494492213 0.2684902131207135  T  T  T
0.3880305016100454  0.1398303066661274 0.2850441862565790  T  T  T
0.4878586198272625  0.1121261659851374 0.2832495420953239  T  T  T
0.5404637264269662  0.2597276287257605 0.2792887684693423  T  T  T
0.6930036738600701  0.3275750813709961 0.2716326439991854  T  T  T
0.7807181652472299  0.2779507779495922 0.2676634760680805  T  T  T
0.6727831140636543  0.4841372745580680 0.2693577578710569  T  T  T
0.8479203625944426  0.3852488203423201 0.2628638584076231  T  T  T
0.7411498542078712  0.5900261105244685 0.2644123144831826  T  T  T
```

0.8288901295195198 0.5419377235937083 0.2614433263056522 T T T

0.1725305875835083 0.6744193421122068 0.2626446982121814 T T T

0.3253902323823414 0.5672867150593169 0.2633823302057197 T T T

0.2179944880265468 0.1118027056036563 0.2740349073315501 T T T

0.0671645252638825 0.2181364035539484 0.2732280792269954 T T T

0.0428421242860449 0.5002835672076067 0.2684035489147875 T T T

0.3641119871410747 0.1360311253101346 0.3148061638778554 T T T

0.3558170985525309 0.0479583122656519 0.2685809605722779 T T T

0.5081806115452137 0.0551016550840120 0.3100414391352912 T T T

0.5283030146791834 0.3364528460350997 0.3037940575698351 T T T

0.5222476915808099 0.3192367679251703 0.2526176684926159 T T T

0.7949444691090425 0.1557917494036782 0.2686223381292372 T T T

0.6049396772583684 0.5245152288054898 0.2712775066226919 T T T

0.9158680045986118 0.3455694387243237 0.2598130629062722 T T T

0.7251588828464228 0.7115456132662810 0.2626278839192185 T T T

0.8816427443836613 0.6255730171359138 0.2578819848745170 T T T

0.5694449457553022 0.0085806020547740 0.2476078345188099 T T T

0.3678680404463888 0.2873631875996208 0.2692389643746615 T T T

0.6316965317946914 0.2150966140878585 0.2778682444712826 T T T

0.5054966488813677 0.0093489639170883 0.2520591911020077 T T T

The following structural data for the epoxy resin on Cu₂O(111) surface is provided in the VASP POSCAR format.

Epoxy resin on Cu$_2$O(111) surface
```
  1.00000000000000
  10.4411001204999998    0.0000000000000000    0.0000000000000000
   0.0000000000000000   18.0846004485999998    0.0000000000000000
   0.0000000000000000    0.0000000000000000   35.0000000000000000
   C   Cu   H   O
  15   72   16   39
Selective dynamics
Direct
  0.5442285857644862  0.3507198127222040  0.2627955288522514   T  T  T
  0.5595413784291026  0.4242472885015118  0.2733020366310370   T  T  T
  0.6835259538552165  0.4547235069458395  0.2754783129788265   T  T  T
  0.7913128235329907  0.4099798141416144  0.2693959503202095   T  T  T
  0.7756749541384949  0.3357268429949940  0.2596729250286458   T  T  T
  0.6515903711391147  0.3049583981519675  0.2550486285093143   T  T  T
  0.6001149430629340  0.5777893939428580  0.2827452706080322   T  T  T
  0.6561244262775929  0.6551026153810326  0.2815787927731250   T  T  T
  0.5552924274197650  0.7170862070104818  0.2811787649589732   T  T  T
  0.3270116612035494  0.7309691003834615  0.2768456900588774   T  T  T
  0.3369796096688518  0.8043212876606205  0.2649817213940864   T  T  T
  0.2053129499632433  0.6976389421622287  0.2808231692934555   T  T  T
  0.2255120213465034  0.8436419085080473  0.2544988703840971   T  T  T
  0.0960342054816863  0.7367552781188493  0.2716249633056194   T  T  T
  0.1035829363088965  0.8098317977655256  0.2570174521624864   T  T  T
  0.0000000000000000  0.0000000000000000  0.0527318339515617   F  F  F
  0.5000000000000000  0.0000000000000000  0.0527318339515617   F  F  F
  0.2500000000000000  0.0833299980000035  0.0527318339515617   F  F  F
  0.7500000000000000  0.0833299980000035  0.0527318339515617   F  F  F
  0.0000000000000000  0.1666699949999995  0.0527318339515617   F  F  F
```

```
0.5000000000000000 0.1666699949999995 0.0527318339515617  F  F  F
0.2500000000000000 0.2500000000000000 0.0527318339515617  F  F  F
0.7500000000000000 0.2500000000000000 0.0527318339515617  F  F  F
0.0000000000000000 0.3333300050000005 0.0527318339515617  F  F  F
0.5000000000000000 0.3333300050000005 0.0527318339515617  F  F  F
0.2500000000000000 0.4166699949999995 0.0527318339515617  F  F  F
0.7500000000000000 0.4166699949999995 0.0527318339515617  F  F  F
0.0000000000000000 0.5000000000000000 0.0527318339515617  F  F  F
0.5000000000000000 0.5000000000000000 0.0527318339515617  F  F  F
0.2500000000000000 0.5833299760000017 0.0527318339515617  F  F  F
0.7500000000000000 0.5833299760000017 0.0527318339515617  F  F  F
0.0000000000000000 0.6666700239999983 0.0527318339515617  F  F  F
0.5000000000000000 0.6666700239999983 0.0527318339515617  F  F  F
0.2500000000000000 0.7500000000000000 0.0527318339515617  F  F  F
0.7500000000000000 0.7500000000000000 0.0527318339515617  F  F  F
0.0000000000000000 0.8333299760000017 0.0527318339515617  F  F  F
0.5000000000000000 0.8333299760000017 0.0527318339515617  F  F  F
0.2500000000000000 0.9166700239999983 0.0527318339515617  F  F  F
0.7500000000000000 0.9166700239999983 0.0527318339515617  F  F  F
0.3333300050000005 0.0000000000000000 0.1230513741155193  F  F  F
0.8333299760000017 0.0000000000000000 0.1230513741155193  F  F  F
0.0833299980000035 0.0833299980000035 0.1230513741155193  F  F  F
0.5833299760000017 0.0833299980000035 0.1230513741155193  F  F  F
0.3333300050000005 0.1666699949999995 0.1230513741155193  F  F  F
0.8333299760000017 0.1666699949999995 0.1230513741155193  F  F  F
0.0833299980000035 0.2500000000000000 0.1230513741155193  F  F  F
0.5833299760000017 0.2500000000000000 0.1230513741155193  F  F  F
0.3333300050000005 0.3333300050000005 0.1230513741155193  F  F  F
0.8333299760000017 0.3333300050000005 0.1230513741155193  F  F  F
0.0833299980000035 0.4166699949999995 0.1230513741155193  F  F  F
0.5833299760000017 0.4166699949999995 0.1230513741155193  F  F  F
0.3333300050000005 0.5000000000000000 0.1230513741155193  F  F  F
0.8333299760000017 0.5000000000000000 0.1230513741155193  F  F  F
```

0.0833299980000035 0.5833299760000017 0.1230513741155193 F F F

0.5833299760000017 0.5833299760000017 0.1230513741155193 F F F

0.3333300050000005 0.6666700239999983 0.1230513741155193 F F F

0.8333299760000017 0.6666700239999983 0.1230513741155193 F F F

0.0833299980000035 0.7500000000000000 0.1230513741155193 F F F

0.5833299760000017 0.7500000000000000 0.1230513741155193 F F F

0.3333300050000005 0.8333299760000017 0.1230513741155193 F F F

0.8333299760000017 0.8333299760000017 0.1230513741155193 F F F

0.0833299980000035 0.9166700239999983 0.1230513741155193 F F F

0.5833299760000017 0.9166700239999983 0.1230513741155193 F F F

0.1713009350462471 0.0049284494727999 0.1911330214648927 T T T

0.7282761341285351 0.9822889594236202 0.1912854037335805 T T T

0.4293614238863057 0.0801243254366355 0.1935768852657418 T T T

0.9246534818626273 0.0734076060268762 0.1922306768194346 T T T

0.2270268449546720 0.1497412708749550 0.1914392517861927 T T T

0.6683110207792069 0.1583053276355884 0.1893480100231244 T T T

0.4285718789205717 0.2342687623783419 0.1912692646956557 T T T

0.9311060599748160 0.2468398368702580 0.1873325151511338 T T T

0.1788851163383498 0.3197245736468233 0.1924214669772653 T T T

0.6697959323389853 0.3205081636295262 0.1955774125760144 T T T

0.4144169880345885 0.4172089848341543 0.1875377965028449 T T T

0.9371917289787035 0.4028666414258169 0.1891786100186650 T T T

0.1723312560202714 0.4542480982207024 0.1897310056944761 T T T

0.6570050573949118 0.4941526587342082 0.1857994551039468 T T T

0.4145844325875458 0.5839120692473756 0.1864835075310722 T T T

0.9177361401763307 0.5718659977861122 0.1876750809904166 T T T

0.1530778834851318 0.6642056173218620 0.1886213165821502 T T T

0.6866151450444704 0.6626999135391642 0.1935135765206653 T T T

0.4289500957588857 0.7554977120673527 0.1856933169712818 T T T

0.9280918520838739 0.7383973521454905 0.1872745470016213 T T T

0.1534709165248316 0.8145144751139597 0.1959254710184481 T T T

0.6872846620123170 0.8376072386382560 0.1884702630521602 T T T

0.4410128915581240 0.9128337945748513 0.1872113023847390 T T T

0.9389060508532268 0.9195700215941827 0.1919820916306207 T T T

0.4482098272899009 0.3271231646857444 0.2612448171448207 T T T

0.4754848439923194 0.4583302436437933 0.2783014732198623 T T T

0.8867163527729147 0.4339382983341196 0.2717599392064471 T T T

0.8606346906964717 0.3013744447468341 0.2562178973836282 T T T

0.6380482883622278 0.2451365642801164 0.2530985819102298 T T T

0.5411050365251953 0.5669644040929498 0.2572604357138246 T T T

0.5411789599420516 0.5712774680281996 0.3086134020514137 T T T

0.7222386606414517 0.6623677179418053 0.3057792607989924 T T T

0.5627388747151443 0.7468686948629255 0.2537325163464814 T T T

0.5730694310789985 0.7570260816871510 0.3043744816502709 T T T

0.4291980479733724 0.8317058900678092 0.2624743304062349 T T T

0.2001552513430624 0.6406718313246884 0.2908476114332927 T T T

0.2327117779443313 0.9028450048016552 0.2486481686075166 T T T

0.0029092555616046 0.7106958603975286 0.2748633495879176 T T T

0.0168203838927781 0.8432299067028524 0.2544474322049410 T T T

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