Adsorption of Aspartic Acid on Ni{100}: A Combined Experimental and Theoretical Study

SUPPORTING INFORMATION

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5 pages / 3 tables

Table S1. Calculated geometric parameters of lowest-energy conformers of aspartic acid in the gas phase. For numbering, refer to **Figure 4** in the article.

Parameters (Å, degrees)	Conformer I	Conformer II	Conformer III
d(O1–C3)	1.220	1.369	1.351
d(O2–C3)	1.374	1.223	1.220
d(O3–C4)	1.224	1.225	1.226
d(O4–C4)	1.369	1.368	1.365
d(N–C1)	1.461	1.464	1.473
d(C1–C2)	1.536	1.535	1.537
d(C1–C3)	1.541	1.542	1.551
d(C2–C4)	1.513	1.514	1.514
∠O1C3O2	122.8	122.7	123.6
∠O3C4O4	122.6	122.5	122.6
∠C3C1C2	113.2	109.6	110.6
∠C1C2C4	113.0	112.4	113.1
∠NC1C2	110.9	111.0	117.1
∠NC1C3	113.6	117.5	109.3
∠O1C3C1	124.8	112.3	113.2
∠O2C3C1	112.3	124.9	123.2
∠O3C4C2	125.8	125.9	125.7
∠O4C4C2	111.5	111.6	111.7
∠(C3C1C2C4)	61.2	65.7	67.6
∠(NC1C2C4)	67.8	65.7	58.5

Table S2. Calculated geometric parameters of aspartic acid adsorbed on Ni{100}. For numbering, refer to **Figure 4** in the article.

Parameters (Å, degrees)	Pentadentate I	Pentadentate II	Tetradentate	Tridentate
d(O1–C3)	1.278	1.304	1.299	1.328
d(O2–C3)	1.287	1.322	1.272	1.324
d(O3–C4)	1.281	1.335	1.310	1.231
d(O4–C4)	1.284	1.333	1.266	1.360
d(N–C1)	1.504	1.499	1.459	1.500
d(C1–C2)	1.546	1.541	1.554	1.524
d(C1–C3)	1.535	1.545	1.548	1.549
d(C2–C4)	1.516	1.534	1.516	1.505
∠O1C3O2	125.0	124.7	123.9	121.3
∠O3C4O4	125.1	120.1	124.8	122.5
∠C3C1C2	118.5	117.3	109.5	112.3
∠C1C2C4	110.6	123.3	111.6	115.7
∠NC1C2	111.2	113.7	111.4	111.1
∠NC1C3	101.4	107.6	115.1	110.3
∠O1C3C1	113.3	115.3	117.8	115.3
∠O2C3C1	121.3	117.6	118.3	119.1
∠O3C4C2	117.5	118.0	114.8	126.4
∠O4C4C2	117.2	115.2	120.3	111.0
∠(C3C1C2C4)	80.2	75.0	44.7	174.6
∠(NC1C2C4)	36.6	51.7	83.8	50.5

Table S3. Calculated vibrational frequencies for the two energetically most stable configurations of aspartic acid adsorbed on Ni{100}.

Pentadentate I (cm^{-1})	Pentadentate II (cm^{-1})
3440.6	3453.2
3357.1	3381.4
3083.9	3068.9
3013.0	2975.8
2983.4	2930.1
1537.7	1564.7
1467.5	1412.1
1460.3	1351.5
1427.9	1335.8
1369.3	1314.3
1345.3	1299.6
1291.6	1265.2
1283.3	1240.3
1265.6	1196.6
1188.3	1174.9
1154.8	1155.4
1055.6	1057.1
1012.5	1034.1
967.3	953.3
934.0	870.8
875.0	808.8
812.2	758.2
775.1	745.4
766.8	737.0
738.7	727.4
722.4	635.8
631.8	600.3
626.4	593.0

606.7	588.9
600.6	588.1
593.9	582.3
585.5	535.1
561.2	515.2
502.6	480.0
479.4	446.0
394.2	422.9
344.8	353.4
294.9	318.5
274.3	294.5
247.6	264.5
227.0	252.0
212.4	228.5
202.2	189.6
166.8	168.5
143.3	153.9
104.4	124.6
100.0	101.6
53.1	97.0