Supporting Information

Predicting and Researching Adsorption Configurations of Pyridazine on Si(100) Surface by Means of X-ray Spectroscopies in Theory

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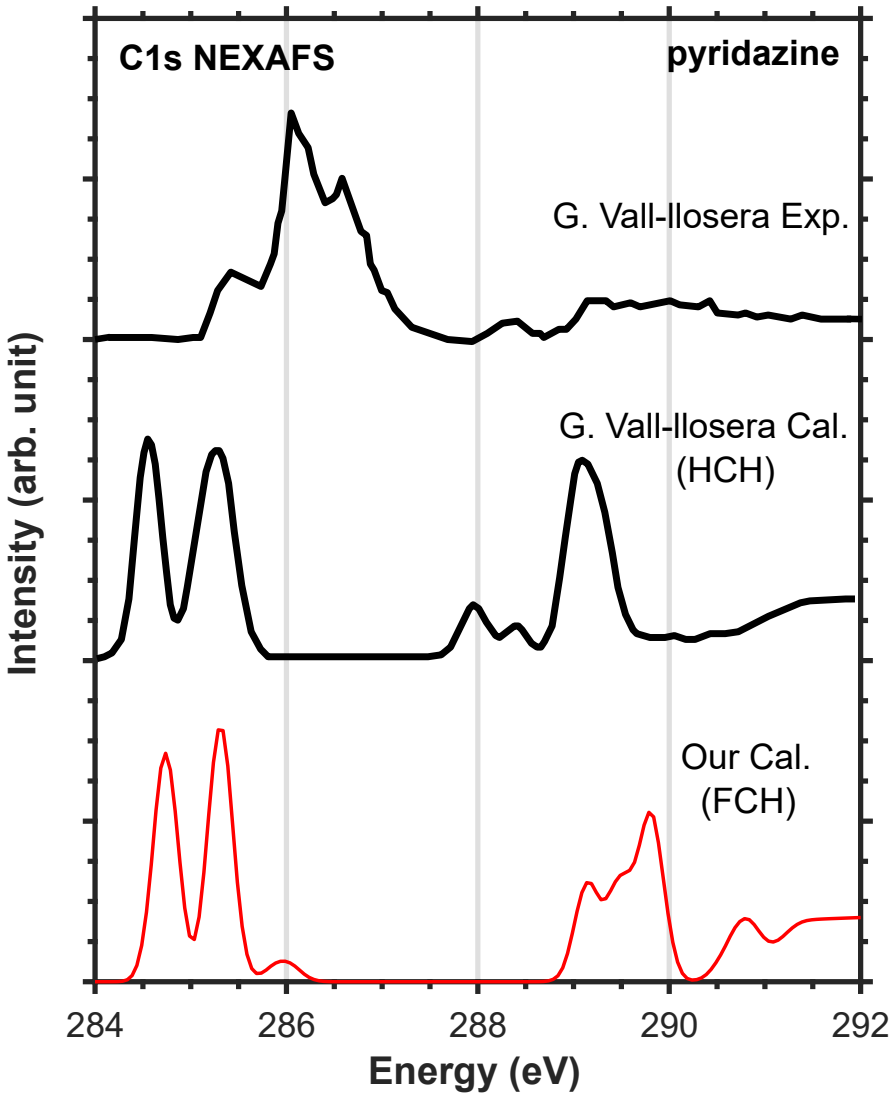

Figure S1 C1s NEXAFS spectra of pyridazine. The spectra in black color, the experimental spectra and calculated spectra in HCH method, were recaptured from the work of G. Vall-llosera et al.[1] The red spectrum is our calculated spectrum in FCH method.

Table S1 The bond lengths of pyridazine ring in each adsorption system. The relative position of C1 to C4 in each adsorption system is the same as that in pyridazine ring shown in Figure 1.

	Bond lengths (Å)					
Adsorption systems	N-N	N-C_1	C_1-C_2	C_2-C_3	C_3-C_4	C_4-N
Mode I	1.4	1.3	1.5	1.6	1.5	1.3
Mode II	1.3	1.5	1.5	1.5	1.4	1.3
Mode III	1.4	1.5	1.5	1.4	1.5	1.3
Mode IV	1.5	1.4	1.4	1.5	1.4	1.4
Mode V	1.2	1.5	1.5	1.3	1.5	1.5
Mode VI	1.5	1.3	1.5	1.5	1.3	1.4
Mode VII	1.2	1.5	1.5	1.3	1.5	1.5
Mode VIII	1.4	1.3	1.5	1.5	1.3	1.4
Mode IX	1.5	1.5	1.6	1.5	1.3	1.4
Mode X	1.4	1.3	1.5	1.6	1.6	1.5
Mode XI	1.2	1.5	1.6	1.6	1.6	1.5
Mode XII	1.5	1.5	1.5	1.3	1.5	1.5
Mode XIII	1.5	1.4	1.3	1.5	1.6	1.5
Mode XIV	1.5	1.3	1.5	1.6	1.6	1.5
Mode XV	1.3	1.5	1.6	1.6	1.6	1.5

Table S2 The bond angles of pyridazine ring in each adsorption system. The relative position of C1 to C4 in each adsorption system is the same as that in pyridazine ring shown in Figure 1.

	Bond angles (°)					
Adsorption systems	N-N-C_1	N-C_1-C_2	C_1-C_2-C_3	C_2-C_3-C_4	C_3-C_4-N	C_4-N-N
Mode I	119.3	128.3	112.2	112.2	128.3	119.3
Mode II	114.8	111.8	107.3	115.7	122.5	121.4
Mode III	122.5	108.9	117.7	120.3	123.2	116.4
Mode IV	113.8	121.7	119.1	118.9	121.6	115.6
Mode V	118.7	110.9	116.9	116.9	110.9	118.7
Mode VI	114.5	123.2	106.6	115.8	120.0	113.3
Mode VII	122.6	115.2	120.5	120.5	115.2	122.6
Mode VIII	113.4	118.2	106.3	111.2	118.4	115.3
Mode IX	117.3	112.2	113.3	118.3	121.3	117.5
Mode X	114.5	124.9	115.2	109.7	113.9	120.6
Mode XI	121.1	120.6	112.2	112.2	120.6	121.1
Mode XII	114.8	111.7	118.2	118.2	111.7	114.8
Mode XIII	111.9	119.9	117.9	107.1	110.6	118.2
Mode XIV	113.3	124.6	108.5	109.5	113.6	111.9
Mode XV	119.3	111.9	111.0	111.0	111.9	119.3

References

1 G. Vall-llosera, B. Gao, A. Kivimäki, M. Coreno, J. Álvarez Ruiz, M. de Simone, H. Ågren and E. Rachlew, *J. Chem. phys.*, 2008, **128**, 044316.