Application of van der Waals functionals to the calculation of dissociative adsorption of N_2 on W(110) for static and dynamic systems

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SUPPLEMENTAL MATERIAL

Parameters					**E_{ads} [eV]**			**E_b^{ext} [eV]**
Supercell	Layers [n]	Kpoints	Cut-off [eV]	Vacuum [Å]	tpv	hlp	bht	hlp to hollow-to-bridge
2x2	5	8x8	450	14	-0.480	-0.626	-0.286	-0.444
3x3	5	8x8	450	14	-0.465	-0.591	-0.248	-0.469
2x2	6	8x8	450	14	-0.486	-0.642	-0.248	-0.393
2x2	7	8x8	450	14	-0.481	-0.596	-0.259	-0.395
3x3	5	8x8	400	13	-0.482	-0.655	-0.236	-0.478
2x2	5	8x8	400	13	-0.475	-0.639	-0.300	-0.447
2x2	5	8x8	450	13	-0.470	-0.615	-0.275	-0.427
2x2	5	8x8	500	13	-0.467	-0.607	-0.267	-0.419
2x2	5	8x8	600	13	-0.466	-0.607	-0.266	-0.417
2x2	5	8x8	400	14	-0.485	-0.650	-0.310	-0.457
2x2	5	8x8	400	15	-0.492	-0.656	-0.317	-0.463
2x2	5	8x8	400	18	-0.499	-0.664	-0.324	-0.470
2x2	5	8x8	400	23	-0.502	-0.667	-0.326	-0.472
2x2	5	4x4	400	13	-0.479	-0.651	-0.313	-0.442
2x2	5	6x6	400	13	-0.455	-0.628	-0.300	-0.443
2x2	5	10x10	400	13	-0.469	-0.630	-0.295	-0.441
2x2	5	11x11	400	13	-0.470	-0.638	-0.298	-0.446
2x2	5	12x12	400	13	-0.470	-0.635	-0.297	-0.446
2x2	8	12x12	600	23	-0.481	-0.608	-0.256	-0.402

Table SI. Convergence tests for N_2 on W(110). Adsorption energies (E_{ads}) for the molecular adsorption states and the dissociation barrier from the hlp molecular adsorption state (E_b^{ext}) are reported. In the first row the results obtained with the setup used for the static and AIMD calculations described in the paper are reported. All the results are for the barrier geometry obtained with the setup reported in the first row of the table.