

SUPPLEMENTARY DOCUMENT

Interaction Energy and Isotheric Heat of Adsorption between Hydrogen and Magnesium Diboride

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1. Fourier series coefficients

Table 1S: The analytical expression of the Fourier series coefficients for 5 terminated planes of MgB₂

n	$g_n^*/2\pi$	$f_n(s_1, s_2)/2$
B (0001) plane		
1	$2/\sqrt{3}$	$-[\cos 2\pi s_1 + \cos 2\pi s_2 + \cos (2\pi(s_1 + s_2))]$
2	2	$2[\cos(2\pi s_1 + s_2) + \cos (s_1 + 2\pi s_2) + \cos (2\pi(s_1 - s_2))]$
3	$4/\sqrt{3}$	$-[\cos(4\pi s_1) + \cos (4\pi s_2) + \cos (4\pi(s_1 + s_2))]$
4	$2\sqrt{7/3}$	$-[\cos 2\pi(3s_1 + s_2) + \cos 2\pi(3s_2 + s_1) + \cos 2\pi(3s_1 + 2s_2) + \cos 2\pi(2s_1 + 3s_2) + \cos 2\pi(s_1 - 2s_2) + \cos 2\pi(2s_1 - s_2)]$
5	$6/\sqrt{3}$	$2[\cos 6\pi s_1 + \cos 6\pi s_2 + \cos (6\pi(s_1 + s_2))]$
Mg (0001) plane		
1	$2/\sqrt{3}$	$\cos 2\pi s_1 + \cos 2\pi s_2 + \cos (2\pi(s_1 + s_2))$
2	2	$\cos 2\pi(2s_1 + s_2) + \cos 2\pi(s_1 + 2\pi s_2) + \cos (2\pi(s_1 - s_2))]$
3	$4/\sqrt{3}$	$\cos(4\pi s_1) + \cos (4\pi s_2) + \cos (4\pi(s_1 + s_2))$
4	$2\sqrt{7/3}$	$\cos 2\pi(3s_1 + s_2) + \cos 2\pi(3s_2 + s_1) + \cos 2\pi(3s_1 + 2s_2) + \cos 2\pi(2s_1 + 3s_2) + \cos 2\pi(s_1 - 2s_2) + \cos 2\pi(2s_1 - s_2)$
5	$6/\sqrt{3}$	$\cos 6\pi s_1 + \cos 6\pi s_2 + \cos (6\pi(s_1 + s_2))$
B (10$\bar{1}$0)		
1	1.317	$-2\cos (2\pi(s_1 + s_2)+\pi)$
2	2	$-2[\cos(4\pi s_1 + \pi) + \cos (4\pi s_2 + \pi)]$
3	2.635	$2\cos 4\pi(s_1 + s_2)$
4	3.034	$2[\cos 2\pi(3s_1 + s_2) + \cos 2\pi(s_1 + 3\pi s_2)]$
5	3.95	$-2\cos (6\pi(s_1 + s_2)+3\pi)$
Mg (10$\bar{1}$0)		
1	1.317	$-2\cos [-2\pi(s_1 + s_2)]$
2	2	$2[\cos(4\pi s_1) + \cos (4\pi s_2)]$
3	2.635	$2\cos 4\pi(s_1 + s_2)$
4	3.034	$-2[\cos 2\pi(3s_1 + s_2) + \cos 2\pi(3s_2 + s_1)]$
5	3.95	$-2\cos 6\pi(s_1 + s_2)$
Mg-B (11$\bar{2}$0) – for Mg		
1	1.193	$2\cos (2\pi(s_1 + s_2)+\pi)$
2	2.16	$-2[\cos(4\pi s_1 + \pi) + \cos (4\pi s_2 + \pi)]$
3	2.38	$2\cos (4\pi(s_1 + s_2))$
4	2.98	$-2[\cos(2\pi(3s_1 + s_2) + 2\pi) + \cos 2\pi(s_1 + 3\pi s_2)]$

5	3.57	$2\cos(6\pi(s_1 + s_2) + 3\pi)$
		Mg-B (11$\bar{2}$0) – for B
1	1.193	$4\cos 2\pi(s_1 + s_2)$
2	2.16	$2[\cos(4\pi s_1) + \cos(4\pi s_2)]$
3	2.38	$4\cos 4\pi(s_1 + s_2)$
4	2.98	$2[\cos 2\pi(3s_1 + s_2) + \cos 2\pi(s_1 + 3\pi s_2)]$
5	3.57	$4\cos 6\pi(s_1 + s_2)$

2. Interaction energies at different charge values

Table 2S: The interaction energy variation at different charge values of B and Mg atoms.

B(0001)		Interaction Energy (kJ mol^{-1}) at varied charge values (q_B : Boron charge, q_{Mg} : Magnesium charge)				
$q_B \backslash q_{Mg}$	1.45	1.55	1.65	1.75	1.85	
-0.2	-33.11	-40.62	-48.88	-57.89	-67.65	
-0.3	-18.73	-22.95	-28.92	-36.24	-44.26	
-0.4	-12.18	-15.14	-18.58	-22.53	-27	
-0.5	-5.49	-9.8	-12.38	-15.3	-18.62	
-0.6	-22.6	-14.41	-4.94	-6.91	-12.77	
Mg(0001)		Interaction Energy at varied charge values				
$q_B \backslash q_{Mg}$	0.68	0.78	0.88	0.98	1.08	
-0.64	-2.39	-1.36	-0.776	-0.1315		
-0.74	-5.28	-3.14	-1.92	-1.15		
-0.84	-9.6	-6.38	-4.0495	-2.56	-1.71	
-0.94	-13.91	-10.8	-7.27	-4.91	-3.35	
-1.04	-19.25	-15.91	-12.08	-8.59	-5.87	
B(101$\bar{0}$)		Interaction Energy at varied charge values				
$q_B \backslash q_{Mg}$	0.83	0.93	1.03	1.13	1.23	
-0.24	-14.35	-18.2	-22.65	-27.71	-33.33	
-0.34	-13.16	-16.75	-20.87	-25.59	-30.85	
-0.44	-11.23	-15.19	-19.36	-23.96	-28.97	
-0.54	-7.89	-12.08	-16.72	-21.73	-27.02	
-0.64	-3.81	-7.99	-12.65	-17.87	-23.57	
Mg(101$\bar{0}$)		Interaction Energy at varied charge values				
$q_B \backslash q_{Mg}$	1.22	1.32	1.42	1.52	1.62	
-1.17	-11.52	-10.69	-8.5	-5.7	-2.95	
-1.27	-11.53	-13.22	-12.47	-10.29	-7.42	
-1.37	-8.61	-13.28	-15.07	-14.39	-12.23	
-1.47	-4.13	-10.36	-15.17	-17.05	-16.46	
-1.57		-5.69	-12.26	-17.19	-19.17	

(1120)	Interaction Energy at varied charge values				
$q_B \backslash q_{Mg}$	1.32	1.42	1.52	1.62	1.72
-0.69	-17.68	-20.64	-22.99	-25.25	-26.9
-0.79	-15.44	-19.77	-23.74	-27.31	-30.68
-0.89	-10.51	-15.99	-21.27	-26.26	-30.99
-0.99	-3.5	-9.72	-16	-22.18	-28.19
-1.09		-1.65	-8.44	-15.48	-22.51