Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Graphitic carbon nitride supported Ni-Co dual-atom catalysts beyond $Ni_1(Co_1)$ single-atom catalysts for hydrogen production: A density functional theory study

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Following the assumption of the inverted mold proposed here, the defect formation energy, $E_{forming}$, for a C_3N_1 fragment in the *g*-CN layer is defined as below,

$$E_{forming} = E(C_3N_4) + E(Frag - C_3N_1) - E(CN)$$

where $E(C_3N_4)$, $E(Frag - C_3N_1)$ and $E(CN)$ are the total energies of *g*-C_3N_4 layer, a C_3N_1 fragment and *g*-CN layer, respectively.

Coordinates of five important structures (.cif), containing pure Co-Ni/*gh*-C_3N_4 (Fig. 1), H-adsorbed Co-Ni/*gh*-C_3N_4 (1H, 2H and 3H adsorption scenarios in Fig. 2), and H_2 adsorption on Co-Ni/*gh*-C_3N_4 (Fig. 5) are illustrated below.

Co-Ni/*gh*-C_3N_4

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CRYSTAL DATA

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data_VESTA_phase_1

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_cell_length_c	20.00000
_cell_angle_alpha	90
_cell_angle_beta	90
_cell_angle_gamma	120
_space_group_name_H-M_alt	'P 1'
_space_group_IT_number	1

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_space_group_symop_operation_xyz
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loop_
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_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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_atom_site_B_iso_or_equiv
_atom_site_type_symbol

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N2	1.0	0.153857	0.482664	0.218987	Biso	1.000000 N
N3	1.0	0.324938	0.494695	0.207750	Biso	1.000000 N
N4	1.0	0.001425	0.170528	0.146783	Biso	1.000000 N
N5	1.0	0.169472	0.172517	0.150115	Biso	1.000000 N
N6	1.0	0.007827	0.340628	0.144807	Biso	1.000000 N
N7	1.0	0.163990	0.330280	0.179028	Biso	1.000000 N

N8	1.0	0.333822	0.340709	0.158525	Biso	1.000000 N
N9	1.0	0.499515	0.998237	0.213011	Biso	1.000000 N
N10	1.0	0.657391	0.488359	0.157773	Biso	1.000000 N
N11	1.0	0.825144	0.493115	0.157165	Biso	1.000000 N
N12	1.0	0.508044	0.172764	0.238203	Biso	1.000000 N
N13	1.0	0.664755	0.167661	0.193042	Biso	1.000000 N
N14	1.0	0.506949	0.339240	0.226691	Biso	1.000000 N
N15	1.0	0.664355	0.331972	0.192886	Biso	1.000000 N
N16	1.0	0.829976	0.332902	0.191659	Biso	1.000000 N
N17	1.0	0.997317	0.500748	0.178542	Biso	1.000000 N
N18	1.0	0.168282	0.001199	0.193186	Biso	1.000000 N
N19	1.0	0.333975	0.000103	0.194426	Biso	1.000000 N
N20	1.0	0.010181	0.674242	0.148317	Biso	1.000000 N
N21	1.0	0.155858	0.672320	0.218938	Biso	1.000000 N
N22	1.0	0.010404	0.841038	0.144561	Biso	1.000000 N
N23	1.0	0.167971	0.837287	0.184901	Biso	1.000000 N
N24	1.0	0.324121	0.833021	0.229849	Biso	1.000000 N
N25	1.0	0.500939	0.501837	0.188450	Biso	1.000000 N
N26	1.0	0.665679	0.992536	0.227527	Biso	1.000000 N
N27	1.0	0.836793	0.002622	0.212896	Biso	1.000000 N
N28	1.0	0.515164	0.675663	0.165069	Biso	1.000000 N
N29	1.0	0.671838	0.670651	0.207921	Biso	1.000000 N
N30	1.0	0.507540	0.833809	0.178356	Biso	1.000000 N
N31	1.0	0.676619	0.838876	0.185095	Biso	1.000000 N
N32	1.0	0.838825	0.836489	0.203620	Biso	1.000000 N
C1	1.0	0.059933	0.120610	0.157720	Biso	1.000000 C
C2	1.0	0.052423	0.277486	0.155708	Biso	1.000000 C
C3	1.0	0.224673	0.278293	0.161223	Biso	1.000000 C
C4	1.0	0.054097	0.437965	0.179696	Biso	1.000000 C
C5	1.0	0.215221	0.435650	0.202106	Biso	1.000000 C
C6	1.0	0.382564	0.442871	0.184228	Biso	1.000000 C
C7	1.0	0.560623	0.120208	0.214605	Biso	1.000000 C
C8	1.0	0.555679	0.279017	0.220039	Biso	1.000000 C
C9	1.0	0.721881	0.276004	0.192627	Biso	1.000000 C
C10	1.0	0.558007	0.438015	0.190928	Biso	1.000000 C
C11	1.0	0.717826	0.441298	0.168541	Biso	1.000000 C
C12	1.0	0.877383	0.439297	0.175535	Biso	1.000000 C
C13	1.0	0.055635	0.620548	0.180446	Biso	1.000000 C
C14	1.0	0.058261	0.782033	0.158098	Biso	1.000000 C
C15	1.0	0.218650	0.782245	0.210781	Biso	1.000000 C
C16	1.0	0.063359	0.944763	0.170660	Biso	1.000000 C
C17	1.0	0.225898	0.951356	0.190838	Biso	1.000000 C
C18	1.0	0.381285	0.941740	0.211663	Biso	1.000000 C
C19	1.0	0.567480	0.620777	0.186763	Biso	1.000000 C

C20	1.0	0.567289	0.784750	0.174994	Biso	1.000000 C
C21	1.0	0.731700	0.779147	0.199624	Biso	1.000000 C
C22	1.0	0.561032	0.939537	0.206344	Biso	1.000000 C
C23	1.0	0.729229	0.950051	0.209935	Biso	1.000000 C
C24	1.0	0.887329	0.945411	0.195807	Biso	1.000000 C
Co1	1.0	0.230334	0.615239	0.274039	Biso	1.000000 Co
Ni1	1.0	0.375752	0.645469	0.199711	Biso	1.000000 Ni

1H-adsorption on Co-Ni/*gh*-C_3N_4

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CRYSTAL DATA

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data_VESTA_phase_1

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_cell_length_b 14.26550
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_cell_angle_alpha 90
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_cell_angle_gamma 120
_space_group_name_H-M_alt 'P 1'
_space_group_IT_number 1

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'x, y, z'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol

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N2	1.0	0.156511	0.485243	0.215404	Biso	1.000000 N

N3	1.0	0.322853	0.484262	0.218693	Biso	1.000000 N
N4	1.0	0.000106	0.170891	0.143184	Biso	1.000000 N
N5	1.0	0.166732	0.170426	0.147279	Biso	1.000000 N
N6	1.0	0.008503	0.341768	0.142260	Biso	1.000000 N
N7	1.0	0.163597	0.330014	0.175575	Biso	1.000000 N
N8	1.0	0.332576	0.337609	0.155978	Biso	1.000000 N
N9	1.0	0.498322	0.001881	0.212185	Biso	1.000000 N
N10	1.0	0.657234	0.490303	0.160360	Biso	1.000000 N
N11	1.0	0.825447	0.495445	0.158431	Biso	1.000000 N
N12	1.0	0.508408	0.174880	0.239065	Biso	1.000000 N
N13	1.0	0.662505	0.168902	0.187639	Biso	1.000000 N
N14	1.0	0.507780	0.340900	0.229870	Biso	1.000000 N
N15	1.0	0.664660	0.333949	0.193356	Biso	1.000000 N
N16	1.0	0.829300	0.333182	0.185007	Biso	1.000000 N
N17	1.0	0.998143	0.501816	0.174257	Biso	1.000000 N
N18	1.0	0.163120	-0.000646	0.193684	Biso	1.000000 N
N19	1.0	0.331010	0.002767	0.195334	Biso	1.000000 N
N20	1.0	0.010446	0.674605	0.141960	Biso	1.000000 N
N21	1.0	0.156270	0.673161	0.212837	Biso	1.000000 N
N22	1.0	0.008541	0.840422	0.139444	Biso	1.000000 N
N23	1.0	0.167293	0.838282	0.178713	Biso	1.000000 N
N24	1.0	0.323290	0.835839	0.225556	Biso	1.000000 N
N25	1.0	0.498425	0.499710	0.192475	Biso	1.000000 N
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N27	1.0	0.833481	0.002056	0.208752	Biso	1.000000 N
N28	1.0	0.503358	0.672854	0.186316	Biso	1.000000 N
N29	1.0	0.667633	0.670183	0.205070	Biso	1.000000 N
N30	1.0	0.504060	0.837687	0.184577	Biso	1.000000 N
N31	1.0	0.669746	0.837707	0.187404	Biso	1.000000 N
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C1	1.0	0.057228	0.119483	0.154466	Biso	1.000000 C
C2	1.0	0.052404	0.277891	0.152324	Biso	1.000000 C
C3	1.0	0.223117	0.276284	0.158680	Biso	1.000000 C
C4	1.0	0.056095	0.439489	0.176287	Biso	1.000000 C
C5	1.0	0.214993	0.434447	0.203075	Biso	1.000000 C
C6	1.0	0.380092	0.436890	0.188049	Biso	1.000000 C
C7	1.0	0.559433	0.122159	0.212760	Biso	1.000000 C
C8	1.0	0.556421	0.281050	0.221559	Biso	1.000000 C
C9	1.0	0.721089	0.277083	0.188733	Biso	1.000000 C
C10	1.0	0.558126	0.439402	0.193877	Biso	1.000000 C
C11	1.0	0.718190	0.443527	0.170162	Biso	1.000000 C
C12	1.0	0.877657	0.440359	0.172422	Biso	1.000000 C
C13	1.0	0.056457	0.621652	0.174762	Biso	1.000000 C
C14	1.0	0.057907	0.782448	0.152156	Biso	1.000000 C

C15	1.0	0.218754	0.783551	0.205026	Biso	1.000000 C
C16	1.0	0.059641	0.943188	0.167875	Biso	1.000000 C
C17	1.0	0.222917	0.951713	0.189276	Biso	1.000000 C
C18	1.0	0.379537	0.944726	0.210172	Biso	1.000000 C
C19	1.0	0.560971	0.619244	0.194212	Biso	1.000000 C
C20	1.0	0.557852	0.783143	0.185139	Biso	1.000000 C
C21	1.0	0.725984	0.778880	0.198241	Biso	1.000000 C
C22	1.0	0.559967	0.942949	0.207231	Biso	1.000000 C
C23	1.0	0.725449	0.950366	0.208628	Biso	1.000000 C
C24	1.0	0.882815	0.944164	0.191952	Biso	1.000000 C
Co1	1.0	0.230043	0.620694	0.278768	Biso	1.000000 Co
Ni1	1.0	0.388340	0.626899	0.266369	Biso	1.000000 Ni
H1	1.0	0.318295	0.622080	0.348238	Biso	1.000000 H

2H-adsorption on Co-Ni/*gh*-C_3N_4

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# CRYSTAL DATA

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_cell_angle_gamma                      120
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_space_group_IT_number                 1

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N3	1.0	0.325133	0.483503	0.216124	Biso	1.000000 N
N4	1.0	0.003001	0.171460	0.137983	Biso	1.000000 N
N5	1.0	0.169864	0.171392	0.141593	Biso	1.000000 N
N6	1.0	0.009983	0.341573	0.140378	Biso	1.000000 N
N7	1.0	0.166552	0.330566	0.170563	Biso	1.000000 N
N8	1.0	0.335907	0.338069	0.152169	Biso	1.000000 N
N9	1.0	0.501460	0.001732	0.213212	Biso	1.000000 N
N10	1.0	0.659335	0.488883	0.159815	Biso	1.000000 N
N11	1.0	0.827831	0.494700	0.159478	Biso	1.000000 N
N12	1.0	0.510441	0.174156	0.240038	Biso	1.000000 N
N13	1.0	0.665613	0.168885	0.190565	Biso	1.000000 N
N14	1.0	0.509361	0.339935	0.229085	Biso	1.000000 N
N15	1.0	0.667029	0.333360	0.194847	Biso	1.000000 N
N16	1.0	0.832122	0.333141	0.189221	Biso	1.000000 N
N17	1.0	0.000560	0.501275	0.176569	Biso	1.000000 N
N18	1.0	0.167986	0.001023	0.187035	Biso	1.000000 N
N19	1.0	0.334879	0.002440	0.191912	Biso	1.000000 N
N20	1.0	0.013752	0.673958	0.144489	Biso	1.000000 N
N21	1.0	0.158406	0.673135	0.218564	Biso	1.000000 N
N22	1.0	0.012076	0.839784	0.138101	Biso	1.000000 N
N23	1.0	0.169685	0.837893	0.181597	Biso	1.000000 N
N24	1.0	0.325751	0.836410	0.229153	Biso	1.000000 N
N25	1.0	0.500917	0.499206	0.191617	Biso	1.000000 N
N26	1.0	0.669702	0.997048	0.225177	Biso	1.000000 N
N27	1.0	0.836443	0.001947	0.202786	Biso	1.000000 N
N28	1.0	0.505749	0.672501	0.198940	Biso	1.000000 N
N29	1.0	0.670822	0.670012	0.197048	Biso	1.000000 N
N30	1.0	0.506270	0.837001	0.189352	Biso	1.000000 N
N31	1.0	0.671328	0.836899	0.185952	Biso	1.000000 N
N32	1.0	0.836189	0.835219	0.190927	Biso	1.000000 N
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C2	1.0	0.055020	0.278414	0.148049	Biso	1.000000 C
C3	1.0	0.226258	0.277025	0.153656	Biso	1.000000 C
C4	1.0	0.058010	0.439020	0.175205	Biso	1.000000 C
C5	1.0	0.217811	0.434330	0.199329	Biso	1.000000 C
C6	1.0	0.382729	0.436682	0.185382	Biso	1.000000 C
C7	1.0	0.562142	0.121755	0.214343	Biso	1.000000 C
C8	1.0	0.558300	0.280208	0.222071	Biso	1.000000 C

C9	1.0	0.723878	0.276946	0.191720	Biso	1.000000 C
C10	1.0	0.560219	0.438425	0.193064	Biso	1.000000 C
C11	1.0	0.720500	0.442552	0.170880	Biso	1.000000 C
C12	1.0	0.880159	0.440053	0.175105	Biso	1.000000 C
C13	1.0	0.059373	0.621390	0.178550	Biso	1.000000 C
C14	1.0	0.060709	0.781871	0.153712	Biso	1.000000 C
C15	1.0	0.220993	0.783689	0.209339	Biso	1.000000 C
C16	1.0	0.063601	0.943919	0.163390	Biso	1.000000 C
C17	1.0	0.226515	0.951943	0.186786	Biso	1.000000 C
C18	1.0	0.382238	0.944386	0.210732	Biso	1.000000 C
C19	1.0	0.563429	0.618723	0.195318	Biso	1.000000 C
C20	1.0	0.559510	0.782391	0.190243	Biso	1.000000 C
C21	1.0	0.728557	0.778730	0.192505	Biso	1.000000 C
C22	1.0	0.563199	0.943131	0.208548	Biso	1.000000 C
C23	1.0	0.728399	0.950088	0.205312	Biso	1.000000 C
C24	1.0	0.885766	0.944164	0.185398	Biso	1.000000 C
Co1	1.0	0.230738	0.614895	0.279671	Biso	1.000000 Co
Ni1	1.0	0.388613	0.617824	0.276751	Biso	1.000000 Ni
H1	1.0	0.300452	0.577734	0.345960	Biso	1.000000 H
H2	1.0	0.426929	0.716392	0.326357	Biso	1.000000 H

3H-adsorption on Co-Ni/*gh*-C_3N_4

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CRYSTAL DATA

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_space_group_name_H-M_alt 'P 1'
_space_group_IT_number 1

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_space_group_symop_operation_xyz

'x, y, z'

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_atom_site_fract_x
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_atom_site_fract_z
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_atom_site_B_iso_or_equiv
_atom_site_type_symbol

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N3	1.0	0.335788	0.996301	0.310065	Biso	1.000000 N
N4	1.0	0.005678	0.166394	0.332625	Biso	1.000000 N
N5	1.0	0.168492	0.176742	0.292187	Biso	1.000000 N
N6	1.0	0.001442	0.330157	0.342922	Biso	1.000000 N
N7	1.0	0.167605	0.334884	0.324728	Biso	1.000000 N
N8	1.0	0.335266	0.341316	0.305320	Biso	1.000000 N
N9	1.0	0.503444	0.001615	0.331236	Biso	1.000000 N
N10	1.0	0.668684	0.997957	0.309020	Biso	1.000000 N
N11	1.0	0.831192	0.995209	0.292898	Biso	1.000000 N
N12	1.0	0.506282	0.168230	0.357549	Biso	1.000000 N
N13	1.0	0.664088	0.175776	0.311280	Biso	1.000000 N
N14	1.0	0.501371	0.331722	0.359801	Biso	1.000000 N
N15	1.0	0.666934	0.335878	0.343118	Biso	1.000000 N
N16	1.0	0.829522	0.341787	0.313217	Biso	1.000000 N
N17	1.0	0.000337	0.500222	0.340498	Biso	1.000000 N
N18	1.0	0.167431	0.494590	0.355847	Biso	1.000000 N
N19	1.0	0.329533	0.489048	0.356587	Biso	1.000000 N
N20	1.0	0.009624	0.667207	0.305862	Biso	1.000000 N
N21	1.0	0.159578	0.676342	0.364882	Biso	1.000000 N
N22	1.0	0.008306	0.832403	0.291260	Biso	1.000000 N
N23	1.0	0.168371	0.834912	0.324218	Biso	1.000000 N
N24	1.0	0.328974	0.839936	0.357799	Biso	1.000000 N
N25	1.0	0.502878	0.499532	0.343086	Biso	1.000000 N
N26	1.0	0.668271	0.498489	0.364278	Biso	1.000000 N
N27	1.0	0.833050	0.496235	0.363111	Biso	1.000000 N
N28	1.0	0.514935	0.675606	0.357667	Biso	1.000000 N
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C2	1.0	0.053067	0.274362	0.333943	Biso	1.000000 C
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C18	1.0	0.383068	0.942395	0.333307	Biso	1.000000 C
C19	1.0	0.565372	0.619168	0.338836	Biso	1.000000 C
C20	1.0	0.562596	0.782891	0.340011	Biso	1.000000 C
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C22	1.0	0.564395	0.943493	0.326953	Biso	1.000000 C
C23	1.0	0.725649	0.946438	0.307182	Biso	1.000000 C
C24	1.0	0.883673	0.939978	0.304697	Biso	1.000000 C
Co1	1.0	0.231255	0.620697	0.413335	Biso	1.000000 Co
Ni1	1.0	0.389124	0.619256	0.409575	Biso	1.000000 Ni
H1	1.0	0.291966	0.575132	0.461467	Biso	1.000000 H
H2	1.0	0.428588	0.713787	0.451943	Biso	1.000000 H
H3	1.0	0.256177	0.696182	0.470382	Biso	1.000000 H

H_2 adsorption on Co-Ni/*gh*-C_3N_4

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CRYSTAL DATA

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   N13       1.0     0.664851   0.168717   0.191570   Biso    1.000000 N
   N14       1.0     0.508054   0.339834   0.231547   Biso    1.000000 N
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   N17       1.0     0.999220   0.500141   0.179135   Biso    1.000000 N
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   N19       1.0     0.336611   0.999915   0.189484   Biso    1.000000 N
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C4	1.0	0.055177	0.436520	0.179708	Biso	1.000000 C
C5	1.0	0.214941	0.432017	0.204297	Biso	1.000000 C
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C13	1.0	0.058432	0.620201	0.180214	Biso	1.000000 C
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C15	1.0	0.220761	0.782233	0.211714	Biso	1.000000 C
C16	1.0	0.065352	0.943278	0.164516	Biso	1.000000 C
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C18	1.0	0.383336	0.942233	0.210855	Biso	1.000000 C
C19	1.0	0.565771	0.620466	0.191021	Biso	1.000000 C
C20	1.0	0.566350	0.785524	0.179855	Biso	1.000000 C
C21	1.0	0.731814	0.779253	0.196508	Biso	1.000000 C
C22	1.0	0.564561	0.942753	0.207231	Biso	1.000000 C
C23	1.0	0.731695	0.951259	0.208006	Biso	1.000000 C
C24	1.0	0.888798	0.944419	0.190682	Biso	1.000000 C
Co1	1.0	0.223015	0.608513	0.278247	Biso	1.000000 Co
Ni1	1.0	0.370758	0.638108	0.208065	Biso	1.000000 Ni
H1	1.0	0.302962	0.613332	0.458623	Biso	1.000000 H
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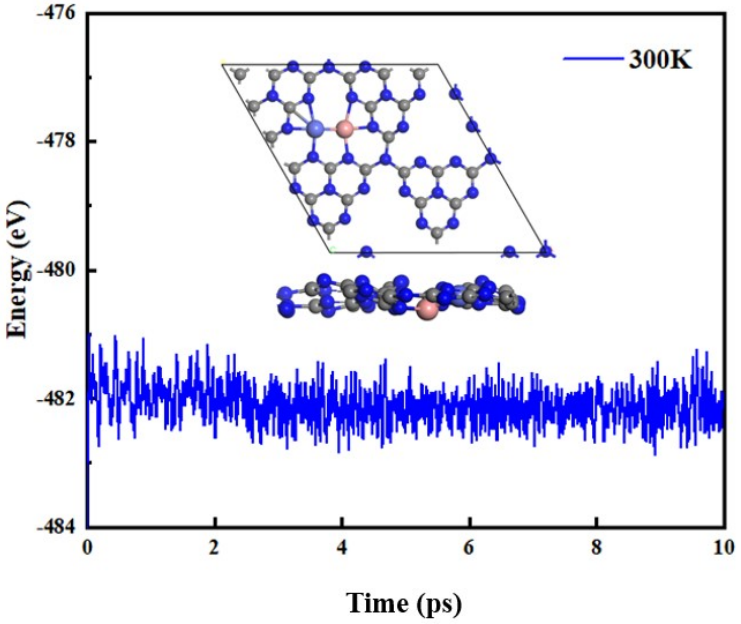

Fig. S1 Molecular dynamic simulation of Ni-Co/*gh*-C_3N_4 monolayer at 300 K. Insets show the top and side views of atomic structures of Ni-Co/*gh*-C_3N_4 monolayer after AIMD run. Blue, gray, purple and pink balls represent N, C, Co and Ni atoms, respectively.