

Supplementary Information

for

Magnetic transition and work function modulation of Ti₂C MXene via porphine adsorption

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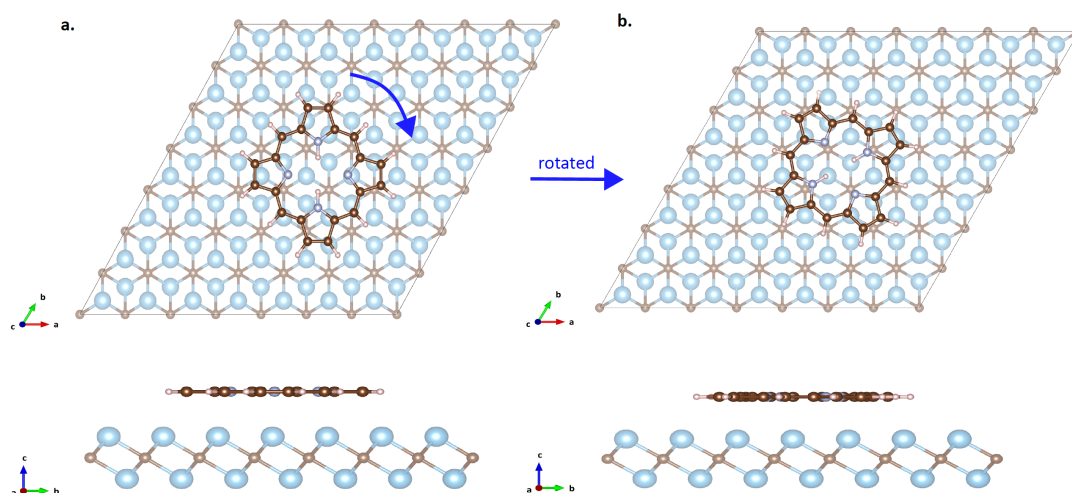


Figure S1. Initial configurations of the porphine molecules on Ti₂C surface **a. Model – I** **b. Model – II**. In Model-I, the corners of the molecule are oriented towards the edges of the substrate, while in Model-II, the corners of the molecule are oriented towards the diagonals of the substrate.

Table S1. Single point energy calculations for different initial distances between the molecule and the substrate for *Model-I* and *Model-II*. (More negative numbers indicate more stability of the structures.)

Distance Between Molecule and Substrate		Relative Total Energy Values (eV) for <i>Porphine</i> + <i>Ti₂C</i> Surfaces			
		2H-P	Cu-P	Ag-P	Au-P
2.6 Å	Model - I	-6.60	-7.04	-8.30	-7.22
3.0 Å		-1.23	-0.86	-1.23	-1.61
3.5 Å		0.00	0.00	0.00	0.00
2.6 Å	Model - II	-7.11	-7.96	-8.22	-7.64
3.0 Å		-0.82	-0.77	-0.64	-1.20
3.5 Å		0.00	0.00	0.00	0.00

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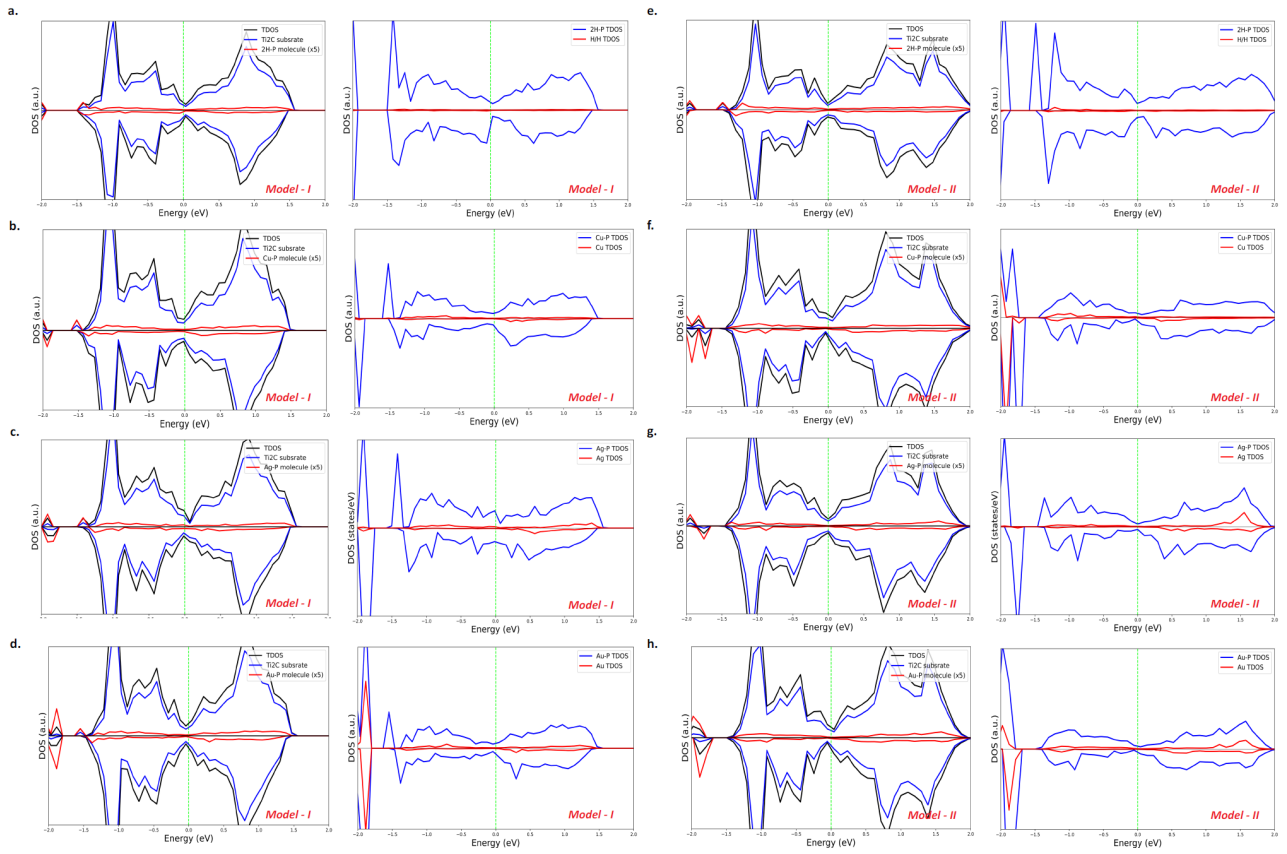


Figure S2. DOS plots of free-based/doped porphine molecules adsorbed on Ti_2C : (a-d) show the data for Model-I, and the right panels, (e-h) show the data for Model-II structures. The plots in the left panel show the contribution of the substrate and the molecule to the total DOS, while those in the right panels show the contribution of each metal atom to the DOS of the molecule.

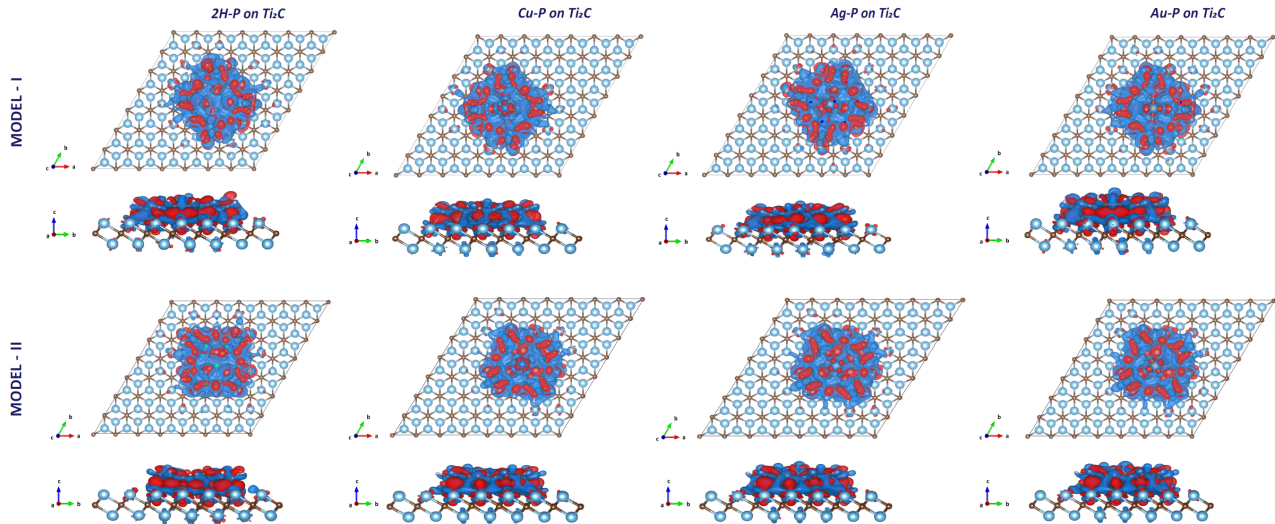


Figure S3. Top and side views of the charge transfer isosurfaces of free-based/doped porphine molecules adsorbed on Ti_2C . Red (blue) color is for charge accumulation (depletion). The isosurface value is $\pm 0.002 \text{ e}/\text{\AA}^3$

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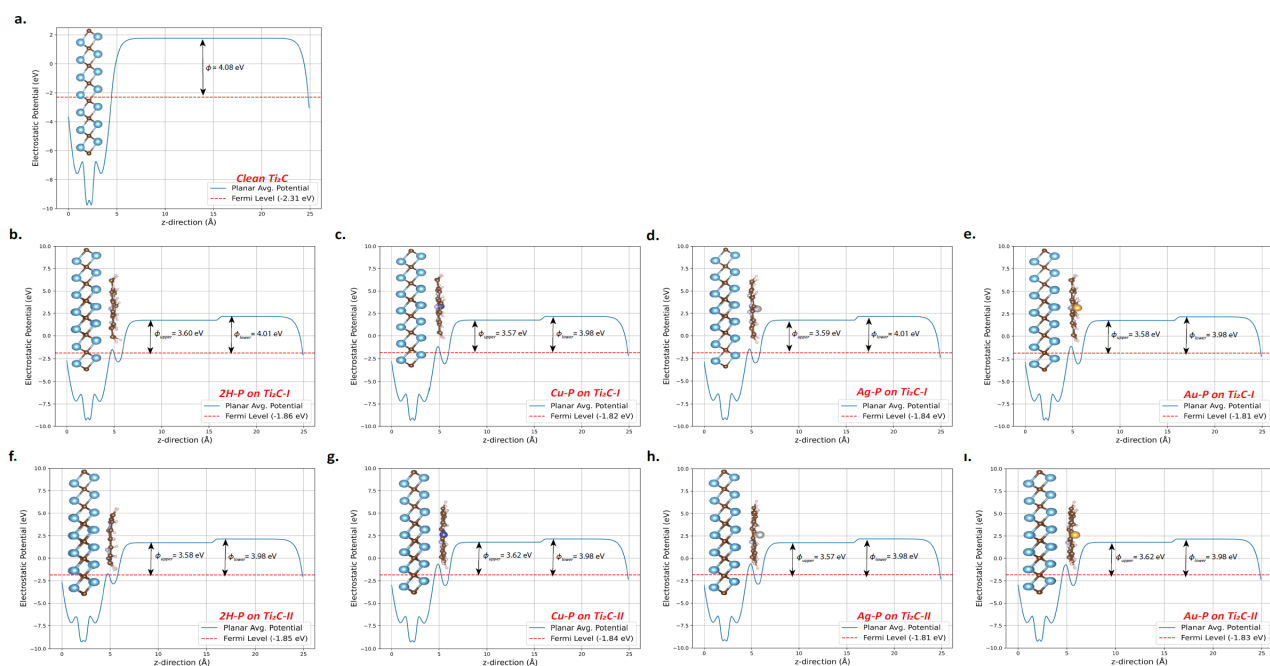


Figure S4. Work function plots of **a.** clean TiC, **b-e.** Porphine+TiC surfaces for *Model-I* **f-i.** Porphine+TiC surfaces for *Model-II*.

Table S2. Cartesian coordinates of the optimized geometries for 2H-P on TiC structure for *Model-I*.

Ti	1.505336999	0.844633208	3.481265903	Ti	15.309131137	8.818584563	3.351998702	Ti	29.073278377	16.747688163	3.432409093
Ti	3.041969004	3.497807657	3.481972218	Ti	16.755783075	11.429316524	3.203533590	Ti	3.048918880	1.726373116	1.041767653
Ti	4.582293407	6.152479451	3.463588282	Ti	18.340056320	14.041506692	3.403892741	Ti	4.581594754	4.367305207	1.031496655
Ti	6.107729324	8.798619958	3.452795744	Ti	19.891054218	16.721110732	3.452403098	Ti	6.116629200	7.015385196	1.012637466
Ti	7.638686034	11.448119431	3.446251899	Ti	13.778000363	0.829901637	3.425703570	Ti	7.641915405	9.673618423	1.001859456
Ti	9.170078383	14.092623604	3.439174592	Ti	15.311338560	3.516797266	3.397765756	Ti	9.170029278	12.321179521	0.994870532
Ti	10.696998318	16.742123078	3.457210213	Ti	16.873915887	6.150206396	3.364156932	Ti	10.704547599	14.990714408	0.994104613
Ti	4.579699569	0.837080721	3.484670445	Ti	18.275098716	8.809419321	3.250301257	Ti	12.235705999	17.646865430	1.028304826
Ti	6.115478459	3.493210653	3.478619084	Ti	19.884951428	11.366267317	3.437835351	Ti	6.105050889	1.723656818	1.033075899
Ti	7.642555132	6.141759747	3.472660109	Ti	21.431842687	14.075913966	3.431186080	Ti	7.637143329	4.364681153	1.023219898
Ti	9.158018042	8.791871048	3.444288671	Ti	22.957354378	16.734879616	3.436750919	Ti	9.165860837	7.013080056	1.022330206
Ti	10.715443545	11.436704921	3.428355604	Ti	16.831149565	0.835086128	3.418431059	Ti	10.682717859	9.650805999	1.010406297
Ti	12.237173090	14.095408360	3.411403298	Ti	18.327860161	3.495327985	3.397464752	Ti	12.206245855	12.336554867	0.961274467
Ti	13.768270807	16.737559265	3.468922153	Ti	19.892623672	6.209483405	3.418666869	Ti	13.778995085	15.014476105	1.010391582
Ti	7.649239321	0.834208147	3.472702950	Ti	21.422494955	8.802215689	3.387235850	Ti	15.290106069	17.652489153	1.032362226
Ti	9.177872711	3.475405423	3.465911746	Ti	22.966808145	11.432608001	3.401076794	Ti	9.161777113	1.711331067	1.013913751
Ti	10.698613283	6.107733621	3.441582993	Ti	24.490086703	14.085373504	3.422771394	Ti	10.684794015	4.353107325	0.998462643
Ti	12.225326497	8.823250716	3.513376415	Ti	26.018969173	16.746252083	3.424249217	Ti	12.210641857	7.023929206	1.033195667
Ti	13.797608468	11.491184119	3.296814859	Ti	19.872928056	0.848047355	3.452726081	Ti	13.697796483	9.636635500	0.957702193
Ti	15.381488231	14.041389416	3.488871455	Ti	21.398942777	3.506831006	3.467186913	Ti	15.261765845	12.370672269	0.861821789
Ti	16.827416445	16.741988099	3.450695425	Ti	22.950619526	6.148419594	3.439792991	Ti	16.820481978	15.016515161	0.989830028
Ti	10.710238144	0.820490917	3.449777886	Ti	24.479278108	8.798275874	3.428484127	Ti	18.355230256	17.630756555	1.024821773
Ti	12.239250044	3.459247037	3.418153524	Ti	26.010605782	11.448668195	3.427715600	Ti	12.224615149	1.703012205	0.990785565
Ti	13.752444051	6.035759256	3.417700529	Ti	27.546809173	14.096280186	3.429528698	Ti	13.746623276	4.339986502	0.963200349

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Ti	15.249135803	7.005398468	0.961900596	C	10.695648122	13.210897250	2.216424979	C	20.403557975	8.096036796	5.487040058
Ti	16.802271978	9.669540311	0.845042430	C	12.233531473	15.871237022	2.229576372	C	20.545083751	9.579633759	5.483132228
Ti	18.412977446	12.337148992	0.928640459	C	16.829045303	18.518541440	2.258957364	C	19.179373311	10.113959390	5.474899709
Ti	19.891227963	14.974936340	1.008733734	C	7.640588524	2.599776322	2.251703478	C	18.377809430	6.533132389	5.346123502
Ti	21.410614507	17.622545012	1.005931757	C	9.168392594	5.244526940	2.243669145	C	17.024233348	6.085200004	5.510639399
Ti	15.297536379	1.714424917	0.979948230	C	10.694825389	7.894152541	2.259702608	C	16.528192561	4.710514968	5.285752192
Ti	16.842054294	4.364462643	0.943372212	C	12.213657162	10.565250187	2.174391970	C	15.022090797	4.805439501	5.376007780
Ti	18.372594847	6.997429222	0.917987060	C	13.769758179	13.243066319	2.166376635	C	14.698879575	6.216984653	5.520074069
Ti	19.915738134	9.682459496	0.912087597	C	15.302086803	15.872440762	2.244012803	C	13.414739500	6.760775907	5.690248311
Ti	21.425240380	12.320829905	0.993070658	C	19.887706435	18.505270426	2.244322374	C	13.073855163	8.156195035	5.636009946
Ti	22.953001812	14.976715397	0.985540636	C	10.698251262	2.586683435	2.224598266	C	11.802038521	8.721245911	5.880796909
Ti	24.478804781	17.624002113	0.983752217	C	12.221158855	5.235079019	2.208271809	C	11.898835201	10.130101456	5.616737530
Ti	18.373494711	1.716586781	0.979321543	C	13.757347554	7.880531358	2.229001373	C	13.318955268	10.403831736	5.441759527
Ti	19.923600570	4.365630979	0.996772945	C	15.256586075	10.555487501	2.049421333	C	13.907270895	11.675736950	5.574995652
Ti	21.442557702	7.014387796	0.981914159	C	16.838578917	13.199815760	2.077422850	C	15.233672825	12.162949654	5.247304216
Ti	22.973679373	9.663427569	0.964700524	C	18.358198611	15.846478478	2.233969793	C	15.633235676	13.549762261	5.593055859
Ti	24.493891844	12.328586727	0.967122056	C	22.951604826	18.503276732	2.217346989	C	17.112408575	13.536096270	5.414163321
Ti	26.019942017	14.979450365	0.980320945	C	13.772037942	2.588576726	2.196925133	C	17.574983343	12.137192049	5.388354883
Ti	27.554482694	17.629395709	0.979777798	C	15.300622746	5.238218922	2.148137987	C	18.863538264	11.506954442	5.573274568
Ti	21.428665774	1.724456730	1.022080518	C	16.808452378	7.907903723	2.057317831	N	18.248986515	9.043138519	5.384670570
Ti	22.958623131	4.365503193	1.022785529	C	18.353267321	10.563846193	2.097987197	N	15.916879048	6.985059907	5.394773558
Ti	24.499223961	7.013274779	0.998863578	C	19.895899274	13.186392066	2.227553725	N	13.976683268	9.160320627	5.191954970
Ti	26.026925029	9.666993427	0.991042051	C	21.424208131	15.850886291	2.223122492	N	16.421919438	11.300373609	5.336325616
Ti	27.552971369	12.323205301	0.986995734	C	26.019201684	18.507854927	2.193575352	H	13.232483316	12.444451138	5.955268070
Ti	29.083381772	14.979554365	0.987610221	C	16.833292153	2.605496023	2.186954021	H	12.645373044	6.098241444	6.082047895
Ti	30.623903874	17.636693383	1.002240088	C	18.393784062	5.253150057	2.153646946	H	19.099216859	5.723144740	5.578242615
C	10.701815699	18.521718960	2.251465432	C	19.887886567	7.917535303	2.139776945	H	19.661601057	12.146461291	5.959894508
C	1.513275299	2.611433682	2.265608869	C	21.442302514	10.540904322	2.177595720	H	17.728217419	14.283320157	5.927555263
C	3.052010175	5.258054634	2.249166183	C	22.962090204	13.203019833	2.201727405	H	15.191713427	14.035312077	6.467054784
C	4.587197175	7.906058836	2.226291597	C	24.485748190	15.858148561	2.208495699	H	16.431605717	10.450934706	5.901944265
C	6.112783923	10.560150888	2.219344489	C	29.080278637	18.513252949	2.206635475	H	11.195759777	10.873322465	6.004262716
C	7.642051651	13.211980394	2.212079242	C	19.885804982	2.609401264	2.224860527	H	10.940036959	8.191304860	6.274607778
C	9.173874559	15.864066581	2.220133878	C	21.422215174	5.263848186	2.230527252	H	14.475013718	4.087016314	5.992584303
C	13.761135129	18.522545425	2.271194197	C	22.965736292	7.904496629	2.200382017	H	17.028119293	3.907607037	5.840638652
C	4.578484433	2.609027308	2.268614061	C	24.493932087	10.560687481	2.191949822	H	15.975203045	7.867745492	5.904456228
C	6.112980876	5.255436942	2.250952832	C	26.020583340	13.210071891	2.200612240	H	21.059640827	7.465618295	6.084360927
C	7.637818347	7.906521856	2.238587849	C	27.550659667	15.863751263	2.205199376	H	21.322592904	10.054581147	6.080292538
C	9.169006770	10.559326635	2.233630605	C	18.969108423	7.852819336	5.439256504				

Table S3. Cartesian coordinates of the optimized geometries for Cu-P on Ti₂C structure for *Model-I*.

Ti	1.596578832	0.862114339	3.447076306	Ti	7.705018905	11.462418271	3.386247158	Ti	6.201179099	3.521564928	3.453167528
Ti	3.126463489	3.516846776	3.440222144	Ti	9.245152157	14.105370194	3.428764269	Ti	7.723448083	6.174568303	3.408700973
Ti	4.656571995	6.172346141	3.419538215	Ti	10.778314773	16.761392877	3.443868458	Ti	9.252985610	8.813167733	3.375829384
Ti	6.190208975	8.817805673	3.393002227	Ti	4.667244013	0.863284749	3.465949744	Ti	10.771905853	11.404196194	3.426864743

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Ti	12.303533109	14.128283299	3.437475115	Ti	12.332814558	17.648035979	1.008408424	C	10.792958920	18.529757908	2.214957774
Ti	13.849954554	16.788597625	3.466778621	Ti	6.199971987	1.744106293	1.018256601	C	1.606521747	2.620597817	2.210821770
Ti	7.745745561	0.869888655	3.461408988	Ti	7.726665718	4.389550888	0.998041872	C	3.132773051	5.275201845	2.202309668
Ti	9.282355687	3.528962454	3.447614610	Ti	9.250198665	7.043759940	0.962194987	C	4.658097687	7.926365865	2.178423293
Ti	10.778537543	6.233716419	3.415393084	Ti	10.778190053	9.711938959	0.923071522	C	6.188037069	10.583270885	2.161559463
Ti	12.388894563	8.804300660	3.252068162	Ti	12.304077978	12.374192767	0.988782477	C	7.721336007	13.227721952	2.183592692
Ti	13.855834095	11.468381652	3.389282152	Ti	13.868617761	15.016384608	1.028678194	C	9.256886257	15.876693682	2.209012955
Ti	15.354479839	14.102431652	3.491356224	Ti	15.390959245	17.658288791	1.025168505	C	13.855380250	18.543552238	2.239705622
Ti	16.926115695	16.776273671	3.469485790	Ti	9.253413026	1.749189412	1.001149602	C	4.669808627	2.629386613	2.239319682
Ti	10.811561534	0.867772152	3.430990502	Ti	10.763493597	4.397599517	0.986131188	C	6.194626296	5.279931061	2.214669064
Ti	12.346210163	3.502001386	3.387197480	Ti	12.325356940	7.022064958	0.918419007	C	7.713000073	7.929293344	2.170871198
Ti	13.830835267	6.153789403	3.354500234	Ti	13.896784239	9.731328247	0.929031800	C	9.246624438	10.570921485	2.176829241
Ti	15.401317189	8.776416596	3.361212090	Ti	15.390837879	12.371083842	0.984684750	C	10.784078217	13.221148955	2.232746221
Ti	16.933288422	11.515260027	3.390201554	Ti	16.903265683	15.018350643	1.021990273	C	12.323398797	15.886902239	2.239333466
Ti	18.478635140	14.132886941	3.424214572	Ti	18.440849452	17.666544589	1.012917981	C	16.921773350	18.547001928	2.254071645
Ti	19.993271165	16.770033695	3.439409658	Ti	12.307074040	1.738892622	0.954513717	C	7.734678105	2.635063719	2.241209336
Ti	13.849839855	0.852577630	3.395801038	Ti	13.841980173	4.383859399	0.938486401	C	9.256977591	5.287748734	2.212096564
Ti	15.369404336	3.512885940	3.393245861	Ti	15.434517799	7.029911396	0.955913961	C	10.793673792	7.937560759	2.132884413
Ti	16.928907431	6.053772209	3.404005989	Ti	16.963868806	9.692718947	1.019443385	C	12.324726796	10.593839015	2.152544819
Ti	18.485178999	8.830028392	3.522531688	Ti	18.446017725	12.361862175	0.990415458	C	13.843353844	13.235409071	2.203105576
Ti	20.012206806	11.476927322	3.414493054	Ti	19.972773736	15.014078915	0.978436507	C	15.384940772	15.900499634	2.267261967
Ti	21.527438163	14.115624113	3.412839025	Ti	21.492275258	17.658941554	0.978895649	C	19.979592585	18.545466274	2.227521501
Ti	23.043994964	16.768319914	3.408327326	Ti	15.377885818	1.737141224	0.953670777	C	10.798778187	2.631987710	2.203775384
Ti	16.905006885	0.851259864	3.398293629	Ti	16.930346736	4.364390729	0.946955662	C	12.295987342	5.270361438	2.161952481
Ti	18.452582664	3.476527014	3.381607309	Ti	18.462832975	7.053021436	1.011834666	C	13.891072056	7.931165336	2.087782137
Ti	19.997474259	6.126780485	3.393774480	Ti	19.970180337	9.685495400	1.001405530	C	15.415494327	10.575493042	2.216914110
Ti	21.537008826	8.812995138	3.401741385	Ti	21.505545665	12.349145457	0.954550505	C	16.917645631	13.261252973	2.232221700
Ti	23.048288125	11.468087356	3.401220962	Ti	23.031158920	15.004894864	0.955051742	C	18.450389454	15.897511305	2.222264931
Ti	24.566492947	14.114220118	3.398616239	Ti	24.562061174	17.650067290	0.953755341	C	23.036351465	18.532701982	2.181656659
Ti	26.094136846	16.767824257	3.402457014	Ti	18.449741264	1.720787701	0.955935102	C	13.844765202	2.623502338	2.173775248
Ti	19.969279874	0.849957034	3.418023139	Ti	19.990741164	4.378132506	0.950678345	C	15.382951649	5.252085167	2.145162784
Ti	21.500440630	3.502365937	3.418698907	Ti	21.510532527	7.042281264	0.968822930	C	16.933960726	7.897743846	2.234409936
Ti	23.035788711	6.162697965	3.420298547	Ti	23.033276436	9.696054679	0.949924346	C	18.469147517	10.594612374	2.228900418
Ti	24.565972032	8.818644861	3.401931748	Ti	24.563928932	12.349382222	0.946525950	C	19.993111473	13.237614084	2.196057327
Ti	26.097001721	11.466657914	3.389101475	Ti	26.096523922	15.002611299	0.953079481	C	21.510153738	15.887050494	2.195773087
Ti	27.621000809	14.108583118	3.399210796	Ti	27.631691870	17.643276337	0.958125480	C	26.095587488	18.528007617	2.169487625
Ti	29.152800533	16.761003431	3.414650634	Ti	21.522717188	1.725995426	0.975163653	C	16.908628301	2.608529437	2.170570195
Ti	3.148549535	1.737121448	1.006568968	Ti	23.045942568	4.381498940	0.972746219	C	18.464213353	5.252771675	2.175836265
Ti	4.668141602	4.382565766	0.994530506	Ti	24.564689705	7.032529642	0.959788449	C	19.998485109	7.918322492	2.219596505
Ti	6.185941126	7.034229040	0.964182802	Ti	26.091839836	9.691241931	0.948005263	C	21.516451991	10.583404757	2.187019028
Ti	7.718059436	9.693439199	0.944547169	Ti	27.626310888	12.352692508	0.941279344	C	23.039827641	13.232919719	2.171011455
Ti	9.267883758	12.351929106	0.983319990	Ti	29.166458672	14.998322974	0.965858437	C	24.565786470	15.883990250	2.177874371
Ti	10.797310937	14.998943653	1.001139637	Ti	30.706589848	17.639634138	0.979494303	C	29.162336701	18.523483634	2.186936513

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C	19.984378555	2.607874738	2.176928706	C	12.256593237	6.415594026	5.398134515	H	15.703773558	14.120817455	6.183405966
C	21.515815139	5.265197968	2.185620554	C	11.642889133	7.714021352	5.436907336	H	13.017343670	14.037541430	5.904908851
C	23.044628942	7.926271823	2.181778103	C	10.219057824	8.021707503	5.472443625	H	9.393604974	10.021820165	6.088968739
C	24.567507311	10.579623154	2.167880535	C	10.142926569	9.516330084	5.482897162	H	9.531295268	7.431320553	6.073954329
C	26.094465173	13.232541338	2.169422805	C	11.526517086	9.980564407	5.457463488	H	13.579236495	3.869483161	5.837668478
C	27.627907169	15.879036993	2.185567841	C	11.987942710	11.335100626	5.487047136	H	16.183548115	4.036095784	5.997360125
C	17.663822570	8.006204924	5.624141172	C	13.338610162	11.841668320	5.618820712	H	19.815230530	7.909071505	6.222330034
C	18.974859572	8.495144685	5.862403288	C	13.703592664	13.233212910	5.614760518	H	19.687427728	10.611964819	6.079144776
C	18.928704745	9.918255367	5.714309588	C	15.136318181	13.296376074	5.754044652	N	16.812543688	9.071523220	5.254224688
C	17.541798702	10.260810152	5.523745343	C	15.604215164	11.939800799	5.645826459	N	14.718781034	6.961867442	5.460701138
C	17.221891189	6.648236165	5.679043010	C	16.975321917	11.548928240	5.696826801	N	12.400485010	8.886418306	5.412677675
C	15.900754305	6.179899943	5.557942763	H	11.224571731	12.079215589	5.760219693	N	14.497491967	11.050944939	5.573550984
C	15.603040151	4.763394895	5.425741151	H	11.580442526	5.580130900	5.645303428	Cu	14.413698050	9.011092811	5.785663426
C	14.115884567	4.669175678	5.314374343	H	17.962189226	5.917199153	6.003545597				
C	13.645203512	6.056923729	5.515769124	H	17.670259436	12.324802912	6.017797813				

Table S4. Cartesian coordinates of the optimized geometries for Ag-P on Ti₂C structure for *Model-I*.

Ti	1.368819284	0.901640550	3.454321623	Ti	16.692194990	11.455026554	3.239256516	Ti	4.428486516	4.424401820	0.978024211
Ti	2.901005183	3.550978838	3.435317427	Ti	18.193172237	14.156843361	3.458060324	Ti	5.960611213	7.083423619	0.964909606
Ti	4.442648004	6.200101866	3.421365097	Ti	19.755335802	16.819726698	3.442825004	Ti	7.501740144	9.747277803	0.986484345
Ti	5.984064142	8.839923291	3.427788988	Ti	13.624195548	0.924541830	3.439540043	Ti	9.036939552	12.390166663	1.019072719
Ti	7.520956364	11.487731111	3.455547616	Ti	15.139926262	3.642554639	3.422183916	Ti	10.550769452	15.040494814	1.002976671
Ti	9.053272692	14.144618981	3.467179462	Ti	16.692556852	6.203702022	3.290390968	Ti	12.084334411	17.688390038	1.013831701
Ti	10.568097473	16.801132896	3.465380520	Ti	18.183947149	8.872072445	3.224382922	Ti	5.956087138	1.768535137	0.991332158
Ti	4.430153141	0.900506166	3.450349346	Ti	19.734064825	11.492218583	3.385426849	Ti	7.471078478	4.413396394	0.950250123
Ti	5.967773081	3.551943600	3.422885388	Ti	21.299712869	14.166202219	3.417584673	Ti	8.989124247	7.074104590	0.917535182
Ti	7.502554733	6.189015397	3.395028785	Ti	22.814794755	16.820711375	3.444410861	Ti	10.535329788	9.747124017	0.935134385
Ti	9.055081204	8.821583403	3.384210914	Ti	16.688638768	0.926310861	3.448429331	Ti	12.074405081	12.405383797	0.953863468
Ti	10.633296053	11.441699115	3.444098681	Ti	18.222523152	3.556687199	3.366556391	Ti	13.628550190	15.066109696	0.991616026
Ti	12.099439041	14.154476816	3.402628005	Ti	19.725564738	6.234990967	3.365592286	Ti	15.145409447	17.691193602	1.011893246
Ti	13.625221889	16.794878537	3.462858498	Ti	21.270206894	8.827187765	3.430053592	Ti	9.020775765	1.767790129	0.968893897
Ti	7.502640488	0.907528491	3.436881304	Ti	22.828883424	11.513810671	3.409597650	Ti	10.529419906	4.397159732	0.911821425
Ti	9.025792729	3.554898461	3.395861760	Ti	24.349741689	14.162753636	3.445446864	Ti	12.070301635	7.070522689	0.858108141
Ti	10.549342763	6.185544134	3.315034136	Ti	25.873365820	16.820917161	3.459533677	Ti	13.602816140	9.736320228	0.876126718
Ti	12.062971132	8.785087839	3.298889473	Ti	19.741351452	0.915174744	3.449627012	Ti	15.146094526	12.424821766	0.912692398
Ti	13.624420554	11.496907416	3.328500688	Ti	21.264860086	3.565099274	3.429311886	Ti	16.692806291	15.073812305	0.996907242
Ti	15.177527665	14.113086080	3.408195451	Ti	22.810039127	6.196037583	3.406347707	Ti	18.215222512	17.701295947	1.002462395
Ti	16.683315475	16.814946035	3.441091999	Ti	24.350765954	8.851271971	3.422933444	Ti	12.098539416	1.771480179	0.974755082
Ti	10.563942686	0.917393655	3.428250924	Ti	25.879278896	11.500774210	3.444349393	Ti	13.619821583	4.397620262	0.913112145
Ti	12.084749451	3.577622099	3.369525075	Ti	27.411390339	14.153294097	3.464956209	Ti	15.141315583	7.070139329	0.861373916
Ti	13.559980671	6.189662076	3.280708939	Ti	28.938067782	16.814624079	3.467271850	Ti	16.690223113	9.748396352	0.826662034
Ti	15.185060018	8.858229434	3.303644061	Ti	2.898592317	1.769918802	1.000970881	Ti	18.259846850	12.446381769	0.920982007

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Ti	19.749707616	15.059965974	1.005697064	C	5.963895742	0.015485679	2.232648805	C	20.679471613	9.049603090	5.680797249
Ti	21.281028264	17.698614085	0.993969757	C	7.491298841	2.661050897	2.196217142	C	19.474562096	9.825466698	5.530309305
Ti	15.158988060	1.778403206	0.998523179	C	9.009600597	5.302314210	2.135216072	C	18.015414896	6.460563345	5.368447676
Ti	16.691105571	4.400070061	0.920129009	C	10.539048377	7.949427225	2.089312300	C	16.572839896	6.350500231	5.453999341
Ti	18.243221633	7.065562793	0.876921602	C	12.085964867	10.596884876	2.118346840	C	15.875746854	5.070881898	5.440628156
Ti	19.814819164	9.756427556	0.906482898	C	13.628925147	13.289868354	2.158069424	C	14.420134278	5.378651027	5.454937741
Ti	21.292313380	12.401775896	0.986347720	C	15.156555631	15.916368425	2.234154195	C	14.335541901	6.825943277	5.343575403
Ti	22.825586103	15.057063943	0.989937689	C	9.032711604	0.021847763	2.220977843	C	13.133927149	7.633531190	5.379223078
Ti	24.349278582	17.699874250	1.004126295	C	10.556240021	2.662120213	2.179201506	C	13.020817929	9.078093450	5.377025157
Ti	18.213256543	1.760736826	0.979221705	C	12.066814600	5.298974606	2.076456137	C	11.817129736	9.863773957	5.522986501
Ti	19.776595281	4.418731905	0.950056594	C	13.629956438	7.968389450	2.089074254	C	12.256433544	11.280067133	5.498765782
Ti	21.314423379	7.078683892	0.959660951	C	15.156128295	10.608424406	2.046033740	C	13.712398721	11.260088145	5.486324057
Ti	22.828279788	9.737593670	0.986629725	C	16.687386982	13.277957080	2.134951577	C	14.518467834	12.460084270	5.415064469
Ti	24.364778929	12.397941187	0.987320207	C	18.218791948	15.942601772	2.229868062	C	15.955798868	12.631543109	5.421477929
Ti	25.888508456	15.048370018	1.011876483	C	12.096564616	0.022567968	2.219511941	C	16.687344185	13.875929363	5.572929978
Ti	27.406157551	17.691028752	1.016949490	C	13.632352776	2.679165914	2.199624106	C	18.089251057	13.500994191	5.695262551
Ti	21.278462732	1.764807608	0.995452516	C	15.138102579	5.318356703	2.089860104	C	18.167182680	12.070298176	5.539680645
Ti	22.813269696	4.420376537	0.982240122	C	16.680307835	7.977470607	2.022088878	C	19.348209298	11.254614889	5.651277676
Ti	24.355188465	7.082488175	0.979278516	C	18.240656979	10.634828136	2.049660683	H	13.977096551	13.332986148	5.796894804
Ti	25.886585126	9.742003696	0.988032483	C	19.753211259	13.291416178	2.217363752	H	12.277693024	7.127409367	5.826053023
Ti	27.419891065	12.392474570	1.013599802	C	21.288086013	15.935487757	2.216251194	H	18.509883355	5.553763128	5.736512691
Ti	28.941562482	15.038132696	1.026300248	C	15.156246772	0.022297379	2.234823070	H	20.223716333	11.762604280	6.060556695
Ti	30.468215651	17.687312425	1.019476354	C	16.676666857	2.679783826	2.210103162	H	18.846182296	14.107927036	6.187751144
C	21.275755981	0.011235464	2.243723907	C	18.237802005	5.309761246	2.111259103	H	16.265942491	14.755468407	6.054760888
C	22.802848514	2.662714061	2.220647410	C	19.755620373	7.967912601	2.102664113	H	11.714162557	12.050763952	6.048284471
C	24.341698321	5.314104336	2.206104062	C	21.298331853	10.617746754	2.203421481	H	10.966914723	9.527215745	6.109525263
C	25.881964916	7.967955197	2.206604369	C	22.828104766	13.283367272	2.204564400	H	13.724123629	4.813495045	6.069953367
C	27.413815741	10.618541134	2.227051556	C	24.349748077	15.933457552	2.228852548	H	16.277841304	4.216883884	5.988425389
C	28.943665945	13.267761800	2.250589989	C	18.216777202	0.014434801	2.237783186	H	20.874110317	6.840157478	6.015229598
C	30.466692828	15.921396917	2.251051739	C	19.742909208	2.664128013	2.192872390	H	21.587277319	9.406994414	6.161832064
C	2.899428532	0.009344730	2.238805220	C	21.277242925	5.321866689	2.188382857	N	18.382577514	8.943332643	5.364868417
C	4.429789123	2.661627321	2.215289511	C	22.827642297	7.963039556	2.198123001	N	15.644561034	7.366460204	5.143861100
C	5.962141541	5.311509324	2.190495096	C	24.356022057	10.624049794	2.204542607	N	14.131074791	9.951648091	5.147494003
C	7.498006066	7.963796872	2.185330354	C	25.884515517	13.275423473	2.232018113	N	16.859906745	11.556649658	5.379813910
C	9.049692237	10.616843949	2.219857275	C	27.410676835	15.927260724	2.252182923	Ag	16.273550219	9.462281268	6.070796773
C	10.570760977	13.252544666	2.238511108	C	18.871811269	7.627292873	5.399104208				
C	12.089083013	15.918612161	2.226874977	C	20.313036872	7.648420282	5.552277714				

Table S5. Cartesian coordinates of the optimized geometries for Au-P on Ti₂C structure for *Model-I*.

Ti	1.476230533	0.876441252	3.439313546	Ti	6.076974158	8.835994540	3.376062587	Ti	10.656919054	16.777983027	3.418135270
Ti	3.017780932	3.530098151	3.431245685	Ti	7.592695769	11.482249004	3.374933824	Ti	4.549010316	0.871583212	3.445377573
Ti	4.558041060	6.187878593	3.398368135	Ti	9.117441817	14.124881184	3.387733549	Ti	6.084827492	3.529088304	3.424025699

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Ti	7.605180492	6.179032542	3.409814835	Ti	7.615577879	9.703437544	0.928125530	Ti	27.514723213	12.362437492	0.914925430
Ti	9.101060370	8.830329880	3.395057097	Ti	9.143101211	12.357756403	0.931300502	Ti	29.049557086	15.020661868	0.930472650
Ti	10.620551352	11.497785881	3.403878957	Ti	10.678875829	15.019890722	0.959527306	Ti	30.590385158	17.671384996	0.961145759
Ti	12.165521515	14.146297358	3.415313736	Ti	12.210355849	17.672719289	0.990971271	C	32.106869778	18.553468711	2.207001671
Ti	13.724674886	16.784954319	3.449437395	Ti	6.075725206	1.747683216	0.990569592	C	22.919353585	2.641991863	2.219016291
Ti	7.615772704	0.872497220	3.435932472	Ti	7.612087012	4.393793851	0.966423750	C	24.456491015	5.290272384	2.194069326
Ti	9.142787895	3.515857120	3.420998529	Ti	9.146142385	7.050768296	0.967352651	C	25.989396765	7.938903903	2.150199004
Ti	10.642389875	6.146737345	3.410189226	Ti	10.686551745	9.691286186	1.004393585	C	27.512196247	10.592585488	2.134892903
Ti	12.148350152	8.841226605	3.538214043	Ti	12.209116799	12.362527109	0.991563033	C	29.040077767	13.245125290	2.139328234
Ti	13.710398100	11.528200234	3.409373760	Ti	13.747413113	15.018588514	1.010550838	C	30.573549147	15.897604241	2.171638608
Ti	15.292707771	14.114994583	3.486788645	Ti	15.263734848	17.664566384	1.007142384	C	13.731158062	18.553583775	2.229868621
Ti	16.799266574	16.797707547	3.453871235	Ti	9.137701624	1.742382140	0.975928735	C	4.549016784	2.638001155	2.217230573
Ti	10.678326488	0.858159657	3.420380875	Ti	10.672368379	4.395076144	0.968541391	C	6.082049809	5.286517334	2.185538039
Ti	12.197330889	3.488666755	3.405404836	Ti	12.197225492	7.063595651	1.039727684	C	7.601921177	7.937763780	2.164737880
Ti	13.728813464	6.071584907	3.445566446	Ti	13.692485765	9.699869473	1.045222394	C	9.127725105	10.595152287	2.167540230
Ti	15.257357068	8.809411577	3.396337107	Ti	15.262587301	12.372694730	1.000100374	C	10.654358153	13.247558217	2.177235484
Ti	16.810243803	11.493950066	3.412241116	Ti	16.783789223	15.023940069	1.016187109	C	12.200562416	15.905227191	2.202539332
Ti	18.347325501	14.142333203	3.425128385	Ti	18.323542248	17.659138490	0.995988958	C	16.797201437	18.552227354	2.222198807
Ti	19.871009676	16.770053610	3.433531895	Ti	12.203630340	1.742288651	0.969426706	C	7.611630452	2.632953025	2.203164622
Ti	13.747095406	0.855941229	3.405798972	Ti	13.728990563	4.387848172	0.983820483	C	9.134648712	5.279094086	2.190725692
Ti	15.290536119	3.510253588	3.416261077	Ti	15.217342080	7.042976070	1.001248602	C	10.647767024	7.930026320	2.226665802
Ti	16.827234076	6.175514810	3.405434638	Ti	16.752635226	9.741385230	0.952234864	C	12.176590728	10.604701442	2.244459093
Ti	18.278553812	8.814529685	3.245213628	Ti	18.342900115	12.383666688	0.980421714	C	13.731848571	13.267820438	2.233671024
Ti	19.887578042	11.430454988	3.413762897	Ti	19.856422129	15.011169138	0.988037419	C	15.266320900	15.908481051	2.251132205
Ti	21.408799128	14.116328876	3.414848447	Ti	21.381961926	17.657205646	0.975517277	C	19.858644403	18.541435736	2.209887840
Ti	22.931883500	16.768804508	3.407222033	Ti	15.271445018	1.758821270	0.965409726	C	10.668314916	2.624120250	2.191909589
Ti	16.803850533	0.854844946	3.395006806	Ti	16.806661273	4.406272421	0.966725126	C	12.191253330	5.270085397	2.213202789
Ti	18.314620255	3.506436858	3.400142118	Ti	18.320037009	7.029691227	0.938725099	C	13.718029142	7.913820636	2.269451320
Ti	19.891345177	6.231815107	3.412888572	Ti	19.868973283	9.720393905	0.920996163	C	15.238665436	10.591802172	2.245319262
Ti	21.414711565	8.825610068	3.368550166	Ti	21.380807033	12.360700477	0.967747625	C	16.807949348	13.249574039	2.199748158
Ti	22.950764846	11.476460430	3.366934136	Ti	22.915357931	15.012969217	0.952074863	C	18.328157348	15.897689432	2.225019969
Ti	24.465111509	14.118986398	3.377923369	Ti	24.449975261	17.662246308	0.953377038	C	22.922958632	18.537828941	2.190023102
Ti	25.990209917	16.773434703	3.387303650	Ti	18.339045709	1.757199318	0.955462456	C	13.743642305	2.622750830	2.194078080
Ti	19.845080682	0.873678348	3.418492153	Ti	19.878686391	4.410304618	0.985700171	C	15.275969811	5.266393411	2.193108387
Ti	21.379412443	3.535595747	3.433774784	Ti	21.396269053	7.052295099	0.951613393	C	16.759044944	7.940960108	2.119354717
Ti	22.933608493	6.186843023	3.391710296	Ti	22.924522975	9.703988521	0.923977140	C	18.329679532	10.611890691	2.157191932
Ti	24.464169646	8.834380886	3.368081152	Ti	24.449643101	12.367132964	0.914992765	C	19.867234556	13.235447795	2.217389084
Ti	25.985442152	11.481755559	3.359157592	Ti	25.980968859	15.020779144	0.929988548	C	21.393920303	15.889638314	2.198749594
Ti	27.514396803	14.124154293	3.369719908	Ti	27.518778113	17.668519475	0.941780210	C	25.988224626	18.540529612	2.166145481
Ti	29.040714619	16.775196058	3.389451280	Ti	21.394676684	1.759966648	0.985702220	C	16.811560304	2.635415271	2.187919803
Ti	3.020196753	1.751756903	0.995197147	Ti	22.922873836	4.398254217	0.979876239	C	18.355524728	5.282496201	2.187582292
Ti	4.549470469	4.392811387	0.974670891	Ti	24.459206418	7.044315342	0.942617748	C	19.867177706	7.944433584	2.134558186
Ti	6.084729760	7.041920032	0.941763539	Ti	25.986185040	9.702763760	0.919466093	C	21.404477223	10.582437782	2.168720402

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C	22.928538272	13.240829221	2.163475752	C	15.135920228	4.688709348	5.464848876	H	19.437337247	12.085692330	5.749040842
C	24.453769543	15.892887748	2.170250379	C	14.813809923	6.098932931	5.625987053	H	17.616604833	14.029464865	5.868789181
C	29.048789286	18.543790110	2.169152163	C	13.481008176	6.572969769	5.717004091	H	14.938747212	14.094261045	6.170925871
C	19.855368641	2.641594120	2.198117413	C	12.985005396	7.918123897	5.611899123	H	10.937739629	10.501279366	6.148912758
C	21.399929833	5.294295730	2.196922712	C	11.671870999	8.399678026	5.885043740	H	10.842113492	7.807987208	6.261049956
C	22.938564376	7.940852236	2.151390724	C	11.708100328	9.825843973	5.778856203	H	14.569377650	3.933581492	6.016011909
C	24.460005836	10.597321895	2.131634951	C	13.078547872	10.193368620	5.532917008	H	17.174414432	3.797080904	5.815770105
C	25.986169070	13.246263754	2.137085609	C	13.666689116	11.485506183	5.711225420	H	21.233327299	7.436549853	6.092569232
C	27.516180882	15.896864074	2.154312469	C	15.035721789	11.903070130	5.673294142	H	21.344146855	10.038092784	6.109960750
C	19.112094743	7.697940690	5.436071008	C	15.502107447	13.266426401	5.741890520	N	18.370505436	8.869137776	5.345020071
C	20.526740887	8.027601183	5.515296757	C	16.940985578	13.209733339	5.595159158	N	16.003721166	6.861489014	5.596008897
C	20.589937407	9.518872543	5.522982404	C	17.330304506	11.822999285	5.634534732	N	13.788200052	9.008252184	5.215997994
C	19.207520627	9.977451057	5.447015911	C	18.691308502	11.322762290	5.475831032	N	16.164262110	11.042077313	5.615740269
C	18.482545358	6.396159930	5.407063663	H	12.967484627	12.259270990	6.030386314	Au	16.140489078	8.948820835	6.068025902
C	17.099251230	5.995538515	5.569706857	H	12.746674955	5.831931093	6.033958122				
C	16.625714563	4.610575773	5.323696136	H	19.173844134	5.561788247	5.625644326				

Table S6. Cartesian coordinates of the optimized geometries for 2H-P on Ti₂C structure for *Model-II*.

Ti	1.421204605	0.691491608	3.466117088	Ti	15.173253722	8.678103942	3.181420139	Ti	28.971260760	16.603647999	3.498379819
Ti	2.942633394	3.348811043	3.481419552	Ti	16.674835020	11.320308318	3.374829308	Ti	2.926533482	1.612933997	1.008989241
Ti	4.475569109	6.011992672	3.488898883	Ti	18.164659658	14.009217317	3.243899951	Ti	4.461927659	4.259275376	1.030361760
Ti	6.007443990	8.659593943	3.482748401	Ti	19.714988274	16.606413211	3.409436823	Ti	5.994144774	6.897962314	1.034774181
Ti	7.549123900	11.306233216	3.471873494	Ti	13.643626892	0.701627008	3.488113362	Ti	7.515410025	9.544830522	1.023158520
Ti	9.081585971	13.942302018	3.467918355	Ti	15.176766382	3.345461067	3.444328880	Ti	9.035939284	12.207483803	0.996632963
Ti	10.610768489	16.598942586	3.467863202	Ti	16.695693419	6.022619599	3.410506743	Ti	10.574362164	14.852600908	1.020904690
Ti	4.473563890	0.701437192	3.426886120	Ti	18.188349258	8.676490403	3.284265491	Ti	12.101224987	17.510740836	1.004559186
Ti	6.001367419	3.355353259	3.464605174	Ti	19.834041177	11.299819573	3.336009554	Ti	5.993301020	1.632918043	0.986793414
Ti	7.536211162	6.012802832	3.473541040	Ti	21.165884240	13.892063570	3.494891129	Ti	7.524979830	4.254007732	1.019640892
Ti	9.087144281	8.662197137	3.454163906	Ti	22.804906612	16.602305816	3.506310295	Ti	9.042267857	6.887075951	1.013636081
Ti	10.610133003	11.300014250	3.369655641	Ti	16.711457577	0.696248235	3.491116839	Ti	10.549076120	9.513946326	0.962096215
Ti	12.210233051	13.923516867	3.421820235	Ti	18.235234811	3.332368023	3.465399770	Ti	12.075155609	12.214737142	0.903794906
Ti	13.681759879	16.602323830	3.382098842	Ti	19.779521143	6.023063455	3.498760534	Ti	13.601369969	14.881390333	0.907698311
Ti	7.508461901	0.702792236	3.428211233	Ti	21.260250361	8.655051964	3.449279156	Ti	15.164233154	17.561665087	0.927008343
Ti	9.056566551	3.352351689	3.465311943	Ti	22.827655596	11.294922967	3.427456620	Ti	9.063258263	1.595761021	1.005960774
Ti	10.599919754	6.020321544	3.426482774	Ti	24.344869210	13.943612184	3.509437170	Ti	10.573751168	4.217222576	1.013849250
Ti	12.215978208	8.657502069	3.346116911	Ti	25.889035337	16.607452982	3.511794291	Ti	12.083883443	6.850685790	0.950665920
Ti	13.630585715	11.308546161	3.265109908	Ti	19.779582442	0.693276128	3.488533235	Ti	13.616306394	9.546882937	0.841167404
Ti	15.195207968	14.032721056	3.259480538	Ti	21.310932708	3.341188684	3.491582482	Ti	15.173518321	12.210439323	0.849811717
Ti	16.699168232	16.616117078	3.321023511	Ti	22.845155841	6.004065006	3.484871549	Ti	16.710132973	14.886112445	0.840694415
Ti	10.565098603	0.695014456	3.469673122	Ti	24.362701157	8.660490505	3.490396279	Ti	18.256535905	17.555918739	0.933236415
Ti	12.116037328	3.353591867	3.455024304	Ti	25.896093368	11.299735658	3.494496960	Ti	12.115568728	1.563952411	1.032455193
Ti	13.628315075	6.052305463	3.425209692	Ti	27.435234032	13.950717702	3.498428367	Ti	13.646467451	4.212280450	1.012216206

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Ti	15.188569024	6.811448443	0.897450595	C	10.600070328	13.080173375	2.218397640	C	19.175075554	6.417907191	5.738197055
Ti	16.733136126	9.538747865	0.855451670	C	12.121479053	15.722372344	2.216468927	C	20.199325836	7.440164293	5.621095258
Ti	18.258799421	12.179527931	0.896851661	C	16.708016312	18.407596343	2.159410031	C	19.475078989	8.693623392	5.467095744
Ti	19.816588550	14.870266726	0.950707833	C	7.526976768	2.480818989	2.230972309	C	16.615594767	6.459463316	5.695045379
Ti	21.317830933	17.486236082	1.033313935	C	9.060838627	5.122805717	2.246914036	C	15.339830748	7.066568908	5.505531279
Ti	15.179840194	1.558120156	1.029622715	C	10.602382331	7.771888526	2.205094598	C	14.039141792	6.484186286	5.640492114
Ti	16.726657361	4.210661982	1.022334877	C	12.098411373	10.419918084	2.082823593	C	13.018040795	7.505075336	5.418885203
Ti	18.274840332	6.817678967	0.959071933	C	13.649142352	13.094344901	2.071110587	C	13.758266343	8.773173162	5.205074574
Ti	19.803607587	9.512986156	0.950150109	C	15.172635998	15.767700320	2.060611110	C	13.192771595	10.101411873	5.377439467
Ti	21.345399472	12.198057987	0.969479674	C	19.768822082	18.384261411	2.219403748	C	13.827913092	11.387450747	5.430652757
Ti	22.825103711	14.835167503	1.083212177	C	10.583196703	2.460547216	2.249312843	C	13.051564485	12.628803552	5.443880417
Ti	24.361094856	17.477608151	1.061837488	C	12.106506079	5.108366972	2.209835789	C	14.033219993	13.737047598	5.444657269
Ti	18.250035006	1.565500679	1.035073587	C	13.650195132	7.763057117	2.038661433	C	15.326775654	13.096228346	5.299421643
Ti	19.789809601	4.222586693	1.051057442	C	15.182067828	10.437091240	2.022411812	C	16.625240744	13.723504620	5.337888888
Ti	21.326488653	6.863008455	1.041848533	C	16.689788052	13.074087647	2.040886513	C	17.889322863	13.011657127	5.187980012
Ti	22.866082469	9.510613762	1.016509886	C	18.233401588	15.765246349	2.079033017	C	19.216182771	13.672680567	5.343068851
Ti	24.374367409	12.203647343	1.042956155	C	22.827703262	18.368388580	2.279673855	C	20.192807496	12.553724856	5.394832287
Ti	25.885413354	14.842977489	1.070990213	C	13.646339984	2.455504329	2.243118921	C	19.444683857	11.301077489	5.463319293
Ti	27.422843747	17.481226607	1.058328686	C	15.173000166	5.107583549	2.219753287	C	20.065338455	10.007292015	5.447441892
Ti	21.306921214	1.585240023	1.040469111	C	16.711189471	7.747833273	2.082227018	N	18.093164631	8.463998985	5.406590769
Ti	22.842949528	4.236840607	1.048893451	C	18.238859521	10.437236584	2.126020378	N	15.180219843	8.493967464	5.329639716
Ti	24.374852390	6.890878896	1.048483502	C	19.761173434	13.080240375	2.113926556	N	15.151057634	11.688515771	5.057135344
Ti	25.904569448	9.543530077	1.040970201	C	21.283189731	15.709615811	2.282355760	N	18.007244198	11.544344445	5.351888936
Ti	27.419211209	12.193013263	1.048128319	C	25.891540633	18.368979608	2.281550579	H	16.663783133	14.663376317	5.888698759
Ti	28.948337548	14.848942929	1.049898308	C	16.711103050	2.448222026	2.249552660	H	12.195322591	10.114634691	5.827066288
Ti	30.486647547	17.494020315	1.043250081	C	18.253645063	5.104565657	2.262556403	H	16.601708520	5.443157514	6.092003621
C	32.024821938	18.376328439	2.261461512	C	19.769354204	7.764925719	2.188910005	H	21.099136783	10.020910167	5.808827331
C	22.842485769	2.468214469	2.265594206	C	21.334731776	10.395606718	2.170130742	H	21.103500548	12.664218515	5.991798632
C	24.372402253	5.125449249	2.276439374	C	22.813868619	13.073485244	2.283928589	H	19.309667296	14.488312833	6.064743768
C	25.904054088	7.778025956	2.271023316	C	24.351258477	15.720404148	2.304151635	H	17.479047295	11.171191276	6.151335416
C	27.432841820	10.426701674	2.268930157	C	28.959927575	18.370010546	2.276636922	H	13.898421167	14.622731007	6.060238115
C	28.959254857	13.077051376	2.260930248	C	19.776527619	2.458210676	2.267068056	H	12.122817941	12.691049538	6.013898712
C	30.492716928	15.725360793	2.264463851	C	21.317746792	5.109801855	2.279511247	H	12.105629676	7.490464184	6.016229282
C	13.648740545	18.391928331	2.206149517	C	22.833631065	7.770121767	2.270195387	H	13.860146846	5.540575762	6.150439434
C	4.467211108	2.483836946	2.238253090	C	24.372065536	10.424906172	2.253236869	H	15.773767905	9.095546163	5.904701705
C	5.999620741	5.131493651	2.257831273	C	25.893182167	13.074570669	2.291594695	H	19.308893921	5.458720660	6.233584169
C	7.531524983	7.779401030	2.253251382	C	27.424158543	15.721628637	2.295828864	H	21.164266825	7.372642514	6.118968298
C	9.062484275	10.431344035	2.215886404	C	17.904496985	7.077438607	5.574333472				

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Table S7. Cartesian coordinates of the optimized geometries for Cu-P on Ti₂C structure for *Model-II*.

Ti	1.376330836	0.799153217	3.333274029	Ti	25.904615700	16.717275694	3.315293494	Ti	22.809289375	14.946898949	0.920050183
Ti	2.912913062	3.450684813	3.379947323	Ti	19.757254167	0.790653484	3.303404178	Ti	24.335795066	17.607137739	0.892150592
Ti	4.448972939	6.118710973	3.404138725	Ti	21.299812906	3.417580053	3.355671707	Ti	18.233938473	1.701181338	0.858595208
Ti	5.978869608	8.784934382	3.383225356	Ti	22.835843251	6.093358345	3.406562871	Ti	19.771533517	4.365001300	0.937791671
Ti	7.507659398	11.443866974	3.337312560	Ti	24.367216187	8.777299020	3.411857646	Ti	21.277648284	7.003741193	1.003928116
Ti	9.034156282	14.086235860	3.296726165	Ti	25.899755638	11.435857089	3.357609422	Ti	22.803344857	9.649068358	0.990554535
Ti	10.558288683	16.719972256	3.299299492	Ti	27.425548154	14.081632842	3.310102759	Ti	24.339649564	12.294973023	0.917472342
Ti	4.435736344	0.809071777	3.377816782	Ti	28.953228143	16.720135167	3.288283193	Ti	25.873010883	14.947273697	0.872390359
Ti	5.974174024	3.460196919	3.408614902	Ti	2.941966357	1.707148158	0.911812267	Ti	27.409180660	17.604972988	0.849602222
Ti	7.501673532	6.125501533	3.418463956	Ti	4.461021905	4.354205510	0.952020457	Ti	21.307488583	1.704304989	0.877104708
Ti	9.018191119	8.798141080	3.402754412	Ti	5.982692869	6.989115352	0.955955740	Ti	22.831153628	4.361068463	0.934472852
Ti	10.519047392	11.459392374	3.338707975	Ti	7.511105691	9.629491570	0.922927146	Ti	24.348816693	7.001502697	0.961404220
Ti	12.058316528	14.089474016	3.323187768	Ti	9.038566945	12.286521265	0.867950097	Ti	25.874081900	9.638555167	0.931896672
Ti	13.602580355	16.744301017	3.346919549	Ti	10.581481626	14.952142269	0.850519390	Ti	27.407309408	12.285265186	0.882245309
Ti	7.510250638	0.804959452	3.408790628	Ti	12.121444100	17.611061676	0.872044706	Ti	28.941425345	14.947774887	0.843703024
Ti	9.045769976	3.446320259	3.425604765	Ti	5.994179742	1.701157739	0.953283032	Ti	30.485786064	17.609399999	0.841146575
Ti	10.549666251	6.099943486	3.450629430	Ti	7.525969705	4.349085041	0.976919678	C	32.012116674	18.488026342	2.077181677
Ti	12.057501401	8.817251365	3.505749831	Ti	9.064976746	6.994615010	0.989589302	C	22.834402093	2.573309460	2.122302093
Ti	13.563470252	11.482031574	3.418258126	Ti	10.597157341	9.613898264	0.975831187	C	24.361399620	5.227874065	2.174105379
Ti	15.093249408	14.101387871	3.436815456	Ti	12.120476407	12.273745639	0.923005085	C	25.885886186	7.881508939	2.173697766
Ti	16.684903939	16.737230649	3.402409463	Ti	13.656870147	14.949540452	0.925401960	C	27.414634765	10.533092116	2.129343165
Ti	10.586837754	0.791346656	3.398018951	Ti	15.184291200	17.605645765	0.928982708	C	28.943111949	13.188783189	2.075755211
Ti	12.120942463	3.419495678	3.417300164	Ti	9.040642853	1.696070983	0.966408348	C	30.475443001	15.838625135	2.052696348
Ti	13.656024806	6.042448213	3.514289722	Ti	10.589111471	4.356517339	0.998351281	C	13.638093376	18.498322777	2.117660785
Ti	15.179902845	8.768144284	3.432553544	Ti	12.127773719	7.002108993	1.070312873	C	4.455509584	2.581065054	2.164964046
Ti	16.693289011	11.461961542	3.549512912	Ti	13.649364688	9.626731426	1.055018769	C	5.983610443	5.230619337	2.189899587
Ti	18.225488676	14.108243363	3.439531887	Ti	15.199452344	12.273449829	1.028107705	C	7.509284358	7.880208031	2.175897584
Ti	19.772218468	16.721476602	3.418198775	Ti	16.699318695	14.937300670	0.995836631	C	9.032992758	10.534706662	2.122802560
Ti	13.660068693	0.786370198	3.353154510	Ti	18.232614413	17.599404736	0.964939827	C	10.562904541	13.191786492	2.078520229
Ti	15.184392803	3.388643598	3.358483695	Ti	12.091390444	1.699598633	0.939838075	C	12.099473176	15.842554934	2.089674956
Ti	16.727637990	6.013724213	3.434676085	Ti	13.623032197	4.373368192	0.992975226	C	16.698476284	18.494958022	2.172239990
Ti	18.268193001	8.741489161	3.546637699	Ti	15.163358419	7.007157448	1.063249695	C	7.514330209	2.577276121	2.195696281
Ti	19.832234156	11.462256999	3.556548278	Ti	16.727783726	9.661285695	1.108255144	C	9.046140755	5.228139326	2.218790206
Ti	21.339006736	14.101220975	3.402854079	Ti	18.238393598	12.279074738	1.085236250	C	10.571182189	7.879846971	2.250924730
Ti	22.847248543	16.718221746	3.366319902	Ti	19.751300020	14.935588390	0.992780043	C	12.084221124	10.541073120	2.205580916
Ti	16.714367311	0.786622182	3.307311865	Ti	21.277133648	17.601188060	0.943217887	C	13.616409385	13.200596321	2.140528299
Ti	18.232529379	3.405440831	3.336159286	Ti	15.154034633	1.696823948	0.883986427	C	15.158063694	15.851082551	2.173853123
Ti	19.754357042	6.033245744	3.450597488	Ti	16.686385149	4.367250312	0.939410541	C	19.759413103	18.486312926	2.184102673
Ti	21.329140250	8.746724125	3.439606194	Ti	18.227293322	7.031266431	1.035700441	C	10.572594603	2.570244729	2.191454854
Ti	22.877003560	11.440822320	3.400951098	Ti	19.748950525	9.664932236	1.088837816	C	12.105053003	5.220955585	2.261948456
Ti	24.382515637	14.084556286	3.350453037	Ti	21.260824710	12.282283960	1.013256116	C	13.627669347	7.871360656	2.348035508

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C	15.153503341	10.549077765	2.306391312	C	24.362217820	10.535980970	2.161560650	C	19.717202684	10.160543953	5.613440081
C	16.692600922	13.205537947	2.259189571	C	25.888518687	13.186786729	2.104840400	C	20.000756233	8.751989289	5.463662670
C	18.223898722	15.846992221	2.197710211	C	27.418205092	15.836693683	2.067237661	H	17.725354346	14.069950178	5.718676945
C	22.822131020	18.484768233	2.144958043	C	17.135343595	6.523849014	5.679637366	H	12.193703196	10.759486364	5.947922259
C	13.635899814	2.562969434	2.144873144	C	18.191493165	5.548741714	5.672493566	H	15.500940807	5.205238132	5.975739611
C	15.169630510	5.201843029	2.225403182	C	19.438074504	6.275774392	5.774041914	H	21.046603153	8.487545617	5.717553048
C	16.711390462	7.854641111	2.313652275	C	19.089778228	7.653654848	5.679721979	H	21.692514108	11.060723685	6.137422253
C	18.255815913	10.544866635	2.331413194	C	15.741422672	6.213611598	5.636447091	H	20.302955837	13.412126148	6.110829058
C	19.768666345	13.203825431	2.271775087	C	14.628770085	7.129721549	5.688330252	H	15.130330762	14.721757877	6.134884252
C	21.297293159	15.840356248	2.168992608	C	13.265465878	6.788593294	5.843634509	H	12.814350852	13.328874436	5.984181536
C	25.888159188	18.481410317	2.087446961	C	12.519707305	8.036428009	5.831857590	H	11.507944510	8.168391680	6.209424837
C	16.703310238	2.560535890	2.095410328	C	13.468542780	9.073819850	5.676329653	H	12.901236258	5.838488718	6.228856141
C	18.236690783	5.199924677	2.154157398	C	13.192532657	10.487735832	5.602422206	H	18.051447824	4.521587797	6.008985117
C	19.776655937	7.864401297	2.269456733	C	14.135886065	11.565645224	5.663364768	H	20.382406233	5.885533755	6.144687082
C	21.312710176	10.531354791	2.272780899	C	13.787772627	12.958063289	5.660999045	N	17.704859883	7.820031229	5.592091758
C	22.831856700	13.191223146	2.160314990	C	15.022765977	13.703392946	5.770445467	N	14.761092704	8.525802431	5.544206752
C	24.358235768	15.838312456	2.108681914	C	16.063957041	12.741269240	5.670280008	N	15.546942418	11.445017509	5.572699881
C	28.950271726	18.483290520	2.057671947	C	17.463838347	13.025461529	5.463277395	N	18.435343301	10.713191873	5.420152059
C	19.766811276	2.566647064	2.097710736	C	18.566850033	12.106453892	5.587887076	Cu	16.561333833	9.590430248	5.744018379
C	21.302736544	5.213612197	2.185164397	C	19.936438989	12.433928206	5.807214099				
C	22.832306063	7.871734149	2.198896005	C	20.658260483	11.202408629	5.833973308				

Table S8. Cartesian coordinates of the optimized geometries for Ag-P on Ti₂C structure for *Model-II*.

Ti	1.392601423	0.796987944	3.329449702	Ti	15.116033664	14.101963168	3.443515085	Ti	21.344799059	8.737683794	3.432742766
Ti	2.930336984	3.443188725	3.373959172	Ti	16.708678706	16.735466845	3.403246538	Ti	22.898266038	11.436963931	3.392814224
Ti	4.468088387	6.109475808	3.405564804	Ti	10.610961957	0.788035078	3.388278251	Ti	24.403856968	14.079542479	3.340074721
Ti	5.994460166	8.779873566	3.389877309	Ti	12.144623688	3.415687169	3.414528247	Ti	25.921042242	16.714045096	3.303001978
Ti	7.524579884	11.441374706	3.345326818	Ti	13.682523235	6.035670044	3.519869826	Ti	19.770987898	0.787534926	3.299347650
Ti	9.049488142	14.084711212	3.299967534	Ti	15.206456252	8.770401478	3.451755347	Ti	21.316180491	3.414986157	3.347477585
Ti	10.573975860	16.716995270	3.300072675	Ti	16.721879117	11.459502966	3.563433068	Ti	22.855292220	6.089627326	3.399355318
Ti	4.455093206	0.802512135	3.373792325	Ti	18.250539559	14.103401383	3.437296055	Ti	24.384470625	8.769197872	3.410719727
Ti	5.996738893	3.449532955	3.411676747	Ti	19.798683660	16.717004289	3.410992934	Ti	25.916302338	11.433672643	3.356447008
Ti	7.523170104	6.120054057	3.429018400	Ti	13.678586632	0.782927564	3.339846429	Ti	27.442102549	14.078254976	3.304617894
Ti	9.035209223	8.796736128	3.417238575	Ti	15.200682290	3.384924786	3.347947294	Ti	28.969406621	16.716975240	3.283578056
Ti	10.537548476	11.461177086	3.353336251	Ti	16.743299319	6.010812173	3.425410215	Ti	2.962411189	1.701962619	0.908256669
Ti	12.077673784	14.08987327	3.333135656	Ti	18.292594782	8.737004709	3.560448150	Ti	4.489777726	4.347037026	0.952921038
Ti	13.620681476	16.743432269	3.348454058	Ti	19.857228582	11.454092888	3.545752454	Ti	6.010263686	6.983296331	0.962513519
Ti	7.536543140	0.797103609	3.406149182	Ti	21.364209376	14.098274626	3.392804688	Ti	7.533922057	9.624726212	0.932968389
Ti	9.070832724	3.440574046	3.428252154	Ti	22.868929669	16.714647633	3.351954249	Ti	9.060671083	12.278321659	0.876587653
Ti	10.575444184	6.096611581	3.462781049	Ti	16.728790168	0.782018627	3.295934363	Ti	10.603288730	14.943681970	0.854089025
Ti	12.074878439	8.818427053	3.523340413	Ti	18.245475486	3.402638631	3.329034215	Ti	12.138526426	17.605761576	0.872130468
Ti	13.585691323	11.484335217	3.431566778	Ti	19.776647744	6.028113913	3.437715848	Ti	6.020402341	1.695615785	0.953168954

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Ti	7.549498124	4.347966255	0.982846908	C	24.383735469	5.220349599	2.169137379	C	22.852261061	7.865145953	2.191792815
Ti	9.088476351	6.993932220	1.004080411	C	25.907303724	7.874014984	2.176814466	C	24.383316734	10.529092963	2.158494835
Ti	10.618192231	9.612635082	0.992129878	C	27.434061544	10.527433398	2.135289231	C	25.909238367	13.180680907	2.097039626
Ti	12.142314281	12.269403262	0.935532933	C	28.962133430	13.182695071	2.077522535	C	27.436503414	15.830886811	2.059208977
Ti	13.678060619	14.944984663	0.933232164	C	30.494201446	15.833498763	2.051814403	C	17.100700514	6.444096418	5.666565518
Ti	15.206302245	17.600516876	0.930280094	C	13.656328026	18.494363617	2.115075150	C	18.143921052	5.456022088	5.668915979
Ti	9.062985391	1.697191587	0.963918060	C	4.477463032	2.574573898	2.163106812	C	19.405382923	6.163380636	5.773601192
Ti	10.609047656	4.359590088	1.002590523	C	6.007296531	5.224720286	2.198372225	C	19.085019020	7.545140920	5.665181876
Ti	12.148071607	7.008433296	1.084866079	C	7.530245151	7.876599274	2.188886265	C	15.687590794	6.168278393	5.607722937
Ti	13.669696539	9.626895811	1.073745879	C	9.052830431	10.532071161	2.137373430	C	14.578984247	7.099995642	5.688597055
Ti	15.219374073	12.269225787	1.040000313	C	10.582435010	13.188550231	2.088907643	C	13.210150669	6.786101295	5.860206484
Ti	16.718821393	14.932561358	0.998841224	C	12.117693715	15.839274705	2.093145817	C	12.485727396	8.048756236	5.863032629
Ti	18.254711115	17.594728728	0.960625905	C	16.721911215	18.490718161	2.170913722	C	13.446917727	9.072429981	5.691455195
Ti	12.108941594	1.699721983	0.929508411	C	7.538221122	2.573317045	2.198070057	C	13.200859942	10.499638505	5.615165614
Ti	13.640226482	4.379219277	0.987225266	C	9.069281052	5.226613571	2.230067225	C	14.150024439	11.580910426	5.671831574
Ti	15.177232131	7.015417130	1.069980113	C	10.590662785	7.880326453	2.270722766	C	13.822021278	12.980518487	5.671155962
Ti	16.747256876	9.660506853	1.120275746	C	12.103964913	10.541073679	2.224479880	C	15.069158391	13.713747896	5.775011356
Ti	18.256596100	12.275731904	1.084525391	C	13.636728720	13.198779605	2.151305359	C	16.101526759	12.739312578	5.669643093
Ti	19.770424434	14.930822811	0.986017639	C	15.179295194	15.849453103	2.178217159	C	17.516615511	12.976907111	5.459981577
Ti	21.296132542	17.597473524	0.930688622	C	19.782672714	18.483411480	2.176454128	C	18.613776719	12.036578927	5.584695920
Ti	15.169829658	1.692850689	0.872283123	C	10.595441423	2.569843833	2.188464919	C	19.986088392	12.337802652	5.820869206
Ti	16.704033996	4.366036983	0.929780096	C	12.126969509	5.221143126	2.267294025	C	20.699128754	11.100044879	5.815161354
Ti	18.241167206	7.032730141	1.034153177	C	13.650180930	7.873550024	2.369662049	C	19.747079210	10.066279993	5.578323817
Ti	19.766696320	9.659738222	1.081872064	C	15.174609316	10.547742801	2.324191400	C	20.005790501	8.645389231	5.455410304
Ti	21.280051903	12.276213197	1.006307197	C	16.714001759	13.202421863	2.264150819	N	17.702475810	7.722591455	5.556658882
Ti	22.829942551	14.940107196	0.907792550	C	18.246675018	15.843433943	2.196427109	N	14.720940144	8.492775876	5.533370680
Ti	24.354026437	17.602133878	0.877008792	C	22.842045497	18.481510641	2.130181040	N	15.557400750	11.456447166	5.562826839
Ti	18.251608402	1.695546428	0.851810063	C	13.654433588	2.562617101	2.132249542	N	18.474396999	10.645986827	5.384819163
Ti	19.788191321	4.358843384	0.928974123	C	15.187528390	5.200433478	2.216599109	H	17.807166318	14.013878969	5.717661533
Ti	21.299966699	6.998892129	0.993059932	C	16.728670080	7.854835567	2.319840434	H	12.205989446	10.783913422	5.963038168
Ti	22.825569306	9.641168691	0.984620568	C	18.279022485	10.545122534	2.329461976	H	15.432770204	5.166214014	5.957836132
Ti	24.363065978	12.286075537	0.909509246	C	19.790556606	13.199753407	2.265444321	H	21.047503669	8.372217382	5.712342257
Ti	25.892078925	14.939555321	0.862462982	C	21.319084626	15.837007273	2.156103285	H	21.730253485	10.944542252	6.122902434
Ti	27.429806919	17.597432513	0.839585810	C	25.905348103	18.476513472	2.072845935	H	20.371823511	13.306462908	6.129387632
Ti	21.322702208	1.697471575	0.871564782	C	16.719164514	2.557039465	2.083811577	H	15.183973734	14.730619822	6.141327244
Ti	22.853772283	4.354133986	0.928281901	C	18.255238698	5.197586203	2.146202346	H	12.856967413	13.368786459	5.998739530
Ti	24.375809568	6.994359457	0.959795541	C	19.798049035	7.859612226	2.257209711	H	11.475281178	8.192379288	6.238999943
Ti	25.897689409	9.629026770	0.933433998	C	21.334513199	10.523822042	2.263136960	H	12.824607428	5.840637280	6.235036878
Ti	27.429572886	12.275430661	0.881441254	C	22.854532013	13.184929188	2.148507968	H	17.992359774	4.425912162	5.993778069
Ti	28.963848241	14.939281522	0.841620875	C	24.377598785	15.833190042	2.095332512	H	20.343033289	5.749650836	6.135241391
Ti	30.504445082	17.601827060	0.837301323	C	28.967220098	18.478144023	2.050609076	Ag	16.586418379	9.565322707	6.394790517
C	32.028048620	18.483566338	2.074946470	C	19.782277245	2.562834708	2.091970884				
C	22.851176001	2.567902440	2.114985748	C	21.322189563	5.208702042	2.173566989				

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Table S9. Cartesian coordinates of the optimized geometries for Au-P on Ti₂C structure for *Model-II*.

Ti	1.389218458	0.781824440	3.351499689	Ti	25.913415605	16.702400510	3.314869131	Ti	22.826678515	14.935578962	0.906554140
Ti	2.926099523	3.433452369	3.401276901	Ti	19.765441692	0.776486219	3.320535570	Ti	24.351811950	17.594154978	0.886445669
Ti	4.464765923	6.104486932	3.421619156	Ti	21.305646208	3.407325133	3.378300254	Ti	18.248723021	1.687959456	0.870190458
Ti	5.990718383	8.773945556	3.393493845	Ti	22.844211281	6.085531047	3.423368096	Ti	19.786163364	4.350434892	0.954338587
Ti	7.520258764	11.430533100	3.341933371	Ti	24.376191280	8.766077463	3.418263000	Ti	21.293739077	6.982101764	1.009262250
Ti	9.044671888	14.068999105	3.301209593	Ti	25.910240048	11.424564989	3.358919201	Ti	22.823178663	9.625533129	0.984329699
Ti	10.571312052	16.703412633	3.312210086	Ti	27.436420436	14.067126763	3.311448627	Ti	24.357824393	12.276945688	0.911428315
Ti	4.452996004	0.787755760	3.387828520	Ti	28.963701230	16.705191002	3.297070439	Ti	25.888985097	14.933357547	0.870271481
Ti	5.994311984	3.442901400	3.421506669	Ti	2.952375450	1.695639159	0.930614866	Ti	27.425619654	17.590802064	0.854431702
Ti	7.519867670	6.113979010	3.431204384	Ti	4.473146372	4.339115710	0.973241357	Ti	21.319389057	1.693038339	0.897747102
Ti	9.028965545	8.789135339	3.405922727	Ti	5.994896981	6.972864286	0.969404404	Ti	22.845392489	4.342751267	0.960009414
Ti	10.532692058	11.446889720	3.334240978	Ti	7.519304662	9.616378352	0.927638874	Ti	24.363334210	6.981514005	0.976783232
Ti	12.075551335	14.072892591	3.325191535	Ti	9.048129632	12.275290900	0.868412484	Ti	25.889300611	9.618011736	0.938579845
Ti	13.619147200	16.726185473	3.351494468	Ti	10.592377756	14.942841698	0.856967891	Ti	27.421008541	12.270311389	0.883566634
Ti	7.528197148	0.787191774	3.407157524	Ti	12.131129748	17.603143868	0.884377330	Ti	28.956731468	14.935623005	0.849574693
Ti	9.065219026	3.433646935	3.427575452	Ti	6.005532339	1.691121519	0.962179782	Ti	30.498734205	17.597361407	0.853927040
Ti	10.571763082	6.094935062	3.451325725	Ti	7.536808715	4.339412184	0.986273217	C	32.022638711	18.475037580	2.095800655
Ti	12.065003815	8.812745761	3.496615463	Ti	9.072223669	6.983098515	0.995311495	C	22.844246459	2.558445300	2.148617323
Ti	13.572712467	11.465481592	3.404304042	Ti	10.601580425	9.601626867	0.970664379	C	24.373390682	5.212457723	2.198541986
Ti	15.119147550	14.087394384	3.422172069	Ti	12.129216912	12.266827219	0.915338594	C	25.897979996	7.865712577	2.188204868
Ti	16.704377732	16.720235044	3.397144025	Ti	13.664743970	14.942084676	0.923978002	C	27.425475286	10.520333374	2.135537317
Ti	10.601641182	0.779365078	3.388252308	Ti	15.195659432	17.596747850	0.932261868	C	28.954560393	13.175473635	2.079321135
Ti	12.134486968	3.408558280	3.409258970	Ti	9.051132320	1.687901753	0.963353148	C	30.487722910	15.825532009	2.063661667
Ti	13.666002362	6.033286260	3.507968466	Ti	10.597580977	4.348141842	0.996302883	C	13.650352752	18.484214203	2.131732112
Ti	15.191501420	8.763754255	3.414567785	Ti	12.133750191	6.992807522	1.060891054	C	4.469007545	2.565742571	2.184199335
Ti	16.708632779	11.452378199	3.541983528	Ti	13.658058059	9.615761440	1.040391702	C	5.998242581	5.217169812	2.208247186
Ti	18.238333425	14.096005338	3.421127748	Ti	15.207250603	12.264726606	1.015930894	C	7.519522942	7.868386787	2.185594569
Ti	19.787228685	16.706344396	3.406787333	Ti	16.711148487	14.932875991	0.980601902	C	9.042843355	10.523377750	2.123570413
Ti	13.669344403	0.775340506	3.347471085	Ti	18.245424964	17.591760686	0.956401084	C	10.574753138	13.180244167	2.080028474
Ti	15.191176502	3.378404433	3.354152445	Ti	12.103830628	1.688255159	0.930468900	C	12.111091899	15.830305041	2.097023382
Ti	16.728304248	6.010087438	3.429604654	Ti	13.634736518	4.363621683	0.984915654	C	16.713722451	18.481943104	2.173209150
Ti	18.281398185	8.736775285	3.528084133	Ti	15.169697454	6.996453003	1.053293618	C	7.529876201	2.565172262	2.201938051
Ti	19.844069278	11.463710148	3.516831506	Ti	16.737842588	9.649958961	1.090197481	C	9.061036264	5.218153705	2.227195209
Ti	21.350351431	14.086115353	3.383198822	Ti	18.248217577	12.272092913	1.055293901	C	10.579493436	7.871521427	2.249751254
Ti	22.858453040	16.704210578	3.354475126	Ti	19.765262491	14.930362247	0.973351503	C	12.091402170	10.530362040	2.189041653
Ti	16.721258272	0.774784942	3.311694084	Ti	21.292042908	17.590759618	0.931041789	C	13.629892434	13.190215826	2.135085013
Ti	18.235928604	3.396547854	3.343831054	Ti	15.168515390	1.682448103	0.881953468	C	15.171659333	15.838737301	2.169541364
Ti	19.756855875	6.033391038	3.458629344	Ti	16.699162002	4.356974186	0.938940261	C	19.773949788	18.473959458	2.175484612
Ti	21.329143018	8.743385091	3.432136516	Ti	18.236844896	7.016505869	1.031867935	C	10.586562353	2.559709533	2.184771139
Ti	22.884092634	11.426985208	3.388448526	Ti	19.764349150	9.647261141	1.064095549	C	12.117044449	5.210638777	2.255116837
Ti	24.391498947	14.068790379	3.342181524	Ti	21.279849134	12.268527167	0.990385780	C	13.635501173	7.863042653	2.335488356

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C	15.162749241	10.538695425	2.289810438	C	24.374939956	10.520212782	2.159994206	C	19.680358548	10.227341557	5.574106552
C	16.708976625	13.195896334	2.233587217	C	25.901374579	13.172833335	2.102314500	C	19.932413671	8.800302591	5.444835681
C	18.239203570	15.835564804	2.182608284	C	27.430395345	15.823052240	2.071558515	H	17.615184136	14.118559466	5.709203246
C	22.835871173	18.472516826	2.134911555	C	17.062377012	6.519494426	5.682850778	H	12.098669463	10.737076504	5.926650094
C	13.647721681	2.551644699	2.135638576	C	18.137681605	5.566731899	5.690021538	H	15.448929251	5.178116601	5.964691770
C	15.176757988	5.191589420	2.217956879	C	19.379828304	6.306313223	5.785951903	H	20.976511990	8.532043614	5.704490604
C	16.717921088	7.844315325	2.299933461	C	19.030098386	7.685044484	5.688178380	H	21.640366480	11.139834966	6.155758152
C	18.270188811	10.534294205	2.293602275	C	15.657586398	6.187898954	5.606085204	H	20.266878788	13.481711731	6.093134783
C	19.781692075	13.197613706	2.236336587	C	14.501748759	7.064682418	5.676901875	H	14.999683964	14.726619107	6.105095084
C	21.312008562	15.828302886	2.153184559	C	13.144390817	6.727716794	5.889373611	H	12.706835684	13.305366906	5.958742796
C	25.900187216	18.467731565	2.087284579	C	12.392651675	7.977238125	5.882782565	H	11.384023962	8.099758372	6.269039805
C	16.713048277	2.549047852	2.097407335	C	13.326107705	9.017824011	5.667127787	H	12.779690891	5.782602171	6.284201215
C	18.244451954	5.190580946	2.161727671	C	13.089118256	10.448315050	5.566829767	H	18.015684415	4.534055391	6.015430380
C	19.788244915	7.851435607	2.257422693	C	14.036788424	11.543581137	5.656705109	H	20.327226413	5.918298469	6.152329190
C	21.325059158	10.517710412	2.246645137	C	13.687154902	12.934867713	5.652625102	N	17.639057174	7.815132340	5.591809751
C	22.845241894	13.178169086	2.143013628	C	14.914611147	13.695903117	5.770277964	N	14.587672176	8.445477204	5.447643195
C	24.371635548	15.824848485	2.101986070	C	15.976292611	12.760333706	5.666421372	N	15.452602121	11.460277331	5.560134109
C	28.961598717	18.470656587	2.069363869	C	17.381398205	13.069810412	5.451803719	N	18.426654983	10.803207656	5.305469361
C	19.776029033	2.554456879	2.116704686	C	18.527032574	12.190164360	5.518444529	Au	16.498732911	9.615371645	6.113754961
C	21.312879326	5.200756490	2.205015045	C	19.899493052	12.511685733	5.764466515				
C	22.841854123	7.857975497	2.208006737	C	20.613938217	11.271766055	5.823545682				

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