

Supporting information

The tesseract in two dimensional materials, a DFT approach

Long Zhou¹, Guanglong zhang¹, Fangyuan Xiu², Shuwei Xia^{1*}, Liangmin Yu¹

¹Key Laboratory of Marine Chemistry Theory and Technology, Ministry of Education, college of Chemistry and Chemical Engineering, Ocean University of China, Qingdao 266100, China

²Molecular Nanofabrication group, MESA+ Institute for Nanotechnology, University of Twente, 7522 NB, Enschede, Netherlands

*Correspondence and requests for materials should be addressed to shuweixia@ouc.edu.cn

POSCAR of C₂₄O₁₂

C24O12

1.0000000000000000		
8.8521003723000007	0.0000000000000000	0.0000000000000000
-4.4260501862000003	7.6661437993000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.0126991272000012

C	O
24	12

Direct

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0.5389605668372255	0.6411037911687174	0.5344220006260443
0.4610394401627715	0.3588962218312801	0.4655779993739557
0.3588962448312785	0.8978567776685082	0.5344220006260443
0.6411037301687230	0.1021432263314921	0.4655779993739557
0.8978567786685048	0.5389605568372247	0.5344220006260443
0.1021432283314923	0.4610394561627729	0.4655779993739557
0.4610394401627715	0.3588962218312801	0.5344220006260443
0.5389605668372255	0.6411037911687174	0.4655779993739557
0.6411037301687230	0.1021432263314921	0.5344220006260443
0.3588962448312785	0.8978567776685082	0.4655779993739557
0.4610394691627704	0.1021432263314921	0.4655779993739557
0.5389605598372285	0.8978567776685082	0.5344220006260443
0.6411037511687212	0.5389605568372247	0.4655779993739557
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0.1021432513314906	0.6411037911687174	0.5344220006260443
0.5389605598372285	0.8978567776685082	0.4655779993739557
0.4610394691627704	0.1021432263314921	0.5344220006260443
0.3588962278312806	0.4610394561627729	0.4655779993739557
0.6411037511687212	0.5389605568372247	0.5344220006260443
0.1021432513314906	0.6411037911687174	0.4655779993739557
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0.7929055393778413	0.5858109707556807	0.4341515718587203
0.5858109427556784	0.7929054913778373	0.5658484281412797
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0.2070944956221581	0.7929054913778373	0.5658484281412797
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0.7929055373778411	0.2070945206221637	0.5658484281412797
0.2070944956221581	0.7929054913778373	0.4341515718587203

POSCAR of C₂₄S₁₂

C24S12

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C	S
24	12

Direct

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0.5346878526162442	0.9063894830561239	0.5332951673257895
0.9063894740561267	0.3717016324398799	0.4667048736742103
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0.3717016464398810	0.4653121483837523	0.4667048736742103
0.6282983775601210	0.5346878506162440	0.5332951673257895
0.5346878526162442	0.9063894830561239	0.4667048736742103
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0.0936105249438768	0.6282983665601165	0.4667048736742103
0.9063894740561267	0.3717016324398799	0.5332951673257895
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0.4653121583837532	0.3717016324398799	0.4667048736742103
0.0936105149438760	0.4653121483837523	0.5332951673257895
0.9063894730561231	0.5346878506162440	0.4667048736742103
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0.4653121583837532	0.3717016324398799	0.5332951673257895
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0.9063894730561231	0.5346878506162440	0.5332951673257895
0.0936105149438760	0.4653121483837523	0.4667048736742103
0.6282983685601167	0.0936105159438725	0.5332951673257895
0.3717016554398782	0.9063894830561239	0.4667048736742103
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0.4071745809121410	0.2035872964560710	0.4234325820607552
0.5928254120878549	0.7964126885439313	0.5765674179392448
0.7964127155439300	0.2035872964560710	0.4234325820607552
0.2035872764560693	0.7964126885439313	0.5765674179392448
0.2035872964560710	0.4071745929121420	0.4234325820607552
0.7964127175439302	0.5928254340878567	0.5765674179392448
0.5928254120878549	0.7964126885439313	0.4234325820607552
0.4071745809121410	0.2035872964560710	0.5765674179392448
0.2035872764560693	0.7964126885439313	0.4234325820607552
0.7964127155439300	0.2035872964560710	0.5765674179392448

POSCAR of C₂₄Se₁₂

C24Se12

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0.0000000000000000	0.0000000000000000	24.1110000609999986

C	Se
24	12

Direct

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0.9100815466178815	0.5332500051871776	0.4673936601249054
0.0899184763821239	0.4667500408128262	0.5326063798750909
0.4667500628128280	0.3768315094307013	0.4673936601249054
0.5332499701871782	0.6231685085692931	0.5326063798750909
0.3768315044307045	0.9100815416178776	0.4673936601249054
0.6231684845692982	0.0899184833821209	0.5326063798750909
0.0899184763821239	0.4667500408128262	0.4673936601249054
0.9100815466178815	0.5332500051871776	0.5326063798750909
0.5332499701871782	0.6231685085692931	0.4673936601249054
0.4667500628128280	0.3768315094307013	0.5326063798750909
0.0899184913821216	0.6231685085692931	0.5326063798750909
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0.5332499661871779	0.9100815416178776	0.5326063798750909
0.4667500468128267	0.0899184833821209	0.4673936601249054
0.3768314934307071	0.4667500408128262	0.5326063798750909
0.6231685055692964	0.5332500051871776	0.4673936601249054
0.9100815416178776	0.3768315094307013	0.5326063798750909
0.0899184913821216	0.6231685085692931	0.4673936601249054
0.4667500468128267	0.0899184833821209	0.5326063798750909
0.5332499661871779	0.9100815416178776	0.4673936601249054
0.6231685055692964	0.5332500051871776	0.5326063798750909
0.3768314934307071	0.4667500408128262	0.4673936601249054
0.4059449914360229	0.2029724747180168	0.4194108365595071
0.5940550045639768	0.7970275162819860	0.5805891634404929
0.7970275042819850	0.2029725157180167	0.4194108365595071
0.2029724887180180	0.7970275162819860	0.5805891634404929
0.7970275212819828	0.5940550415639763	0.4194108365595071
0.2029725157180167	0.4059450314360262	0.5805891634404929
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0.4059449914360229	0.2029724747180168	0.5805891634404929
0.2029724887180180	0.7970275162819860	0.4194108365595071
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0.2029725157180167	0.4059450314360262	0.4194108365595071
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POSCAR of C₁₆S₁₆

C16S16

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1.0000000000000000
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C S
16 16

Direct

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0.6112107864016920	0.5666576623990665	0.4649202068973324
0.3887892405983067	0.4333423096009312	0.5350798361026676
0.5666576623990665	0.3887892405983067	0.4649202068973324
0.4333423096009312	0.6112107864016920	0.5350798361026676
0.4333423096009312	0.6112107864016920	0.4649202068973324
0.5666576623990665	0.3887892405983067	0.5350798361026676
0.1403166398713438	0.2056341841463123	0.5349050261131651
0.8596834011286560	0.7943658298536818	0.4650949738868349
0.8596834011286560	0.7943658298536818	0.5349050261131651
0.1403166398713438	0.2056341841463123	0.4650949738868349
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0.2056341841463123	0.8596834011286560	0.5349050261131651
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0.2378800930006477	0.3640973409493071	0.4207170163627296
0.7621198789993500	0.6359026860506916	0.5792829836372704
0.7621198789993500	0.6359026860506916	0.4207170163627296
0.2378800930006477	0.3640973409493071	0.5792829836372704
0.6359026860506916	0.2378800930006477	0.4207170163627296
0.3640973409493071	0.7621198789993500	0.5792829836372704
0.3640973409493071	0.7621198789993500	0.4207170163627296
0.6359026860506916	0.2378800930006477	0.5792829836372704
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0.0499078139049800	0.7460953438631535	0.4326251239769405
0.0499078139049800	0.7460953438631535	0.5673748760230595
0.9500921550950139	0.2539046561368465	0.4326251239769405
0.7460953438631535	0.9500921550950139	0.5673748760230595
0.2539046561368465	0.0499078139049800	0.4326251239769405
0.2539046561368465	0.0499078139049800	0.5673748760230595
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POSCAR of C₁₆Se₁₆

C16Se16

1.0000000000000000

9.1443996428999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.1443996428999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.0608997345000013

C	Se
16	16

Direct

0.4403342079034260	0.6062380814236477	0.4658399536128925
0.5596657920965740	0.3937619185763523	0.5341600053871076
0.5596657920965740	0.3937619185763523	0.4658399536128925
0.4403342079034260	0.6062380814236477	0.5341600053871076
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0.1416263714101618	0.2112306190408475	0.4667185119633501
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0.3699027724508213	0.7584725234560636	0.5837643903237790
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0.7584725234560636	0.6300972275491787	0.5837643903237790
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0.7383882269644673	0.9461140555551566	0.5686997162782248
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0.2616117730355327	0.0538859474448401	0.5686997162782248
0.7383882269644673	0.9461140555551566	0.4313002837217752
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0.9461140555551566	0.2616117730355327	0.4313002837217752
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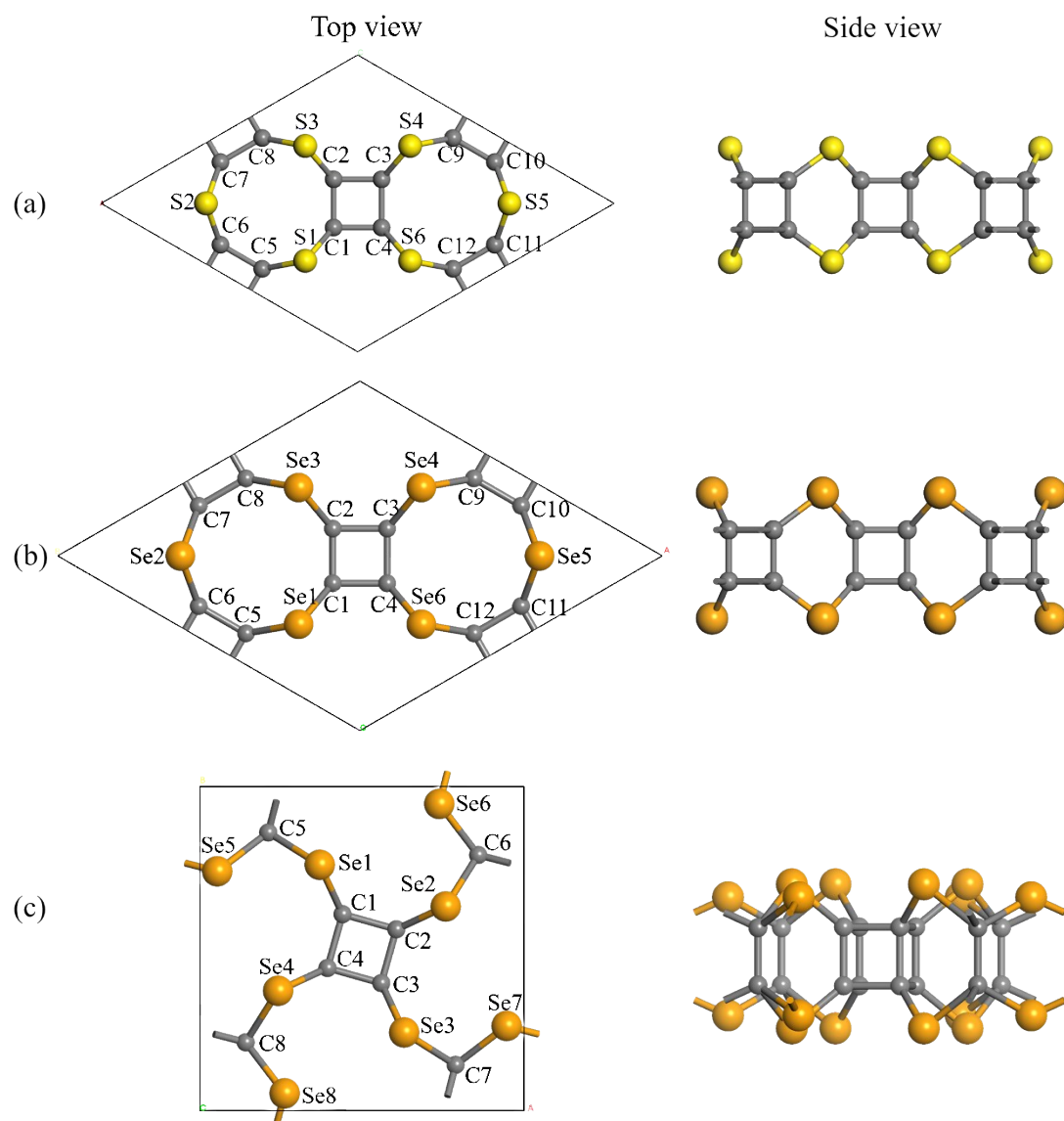


Fig. S1 Snapshot of (a) $C_{24}S_{12}$ (b) $C_{24}Se_{12}$ and (c) $C_{16}Se_{16}$

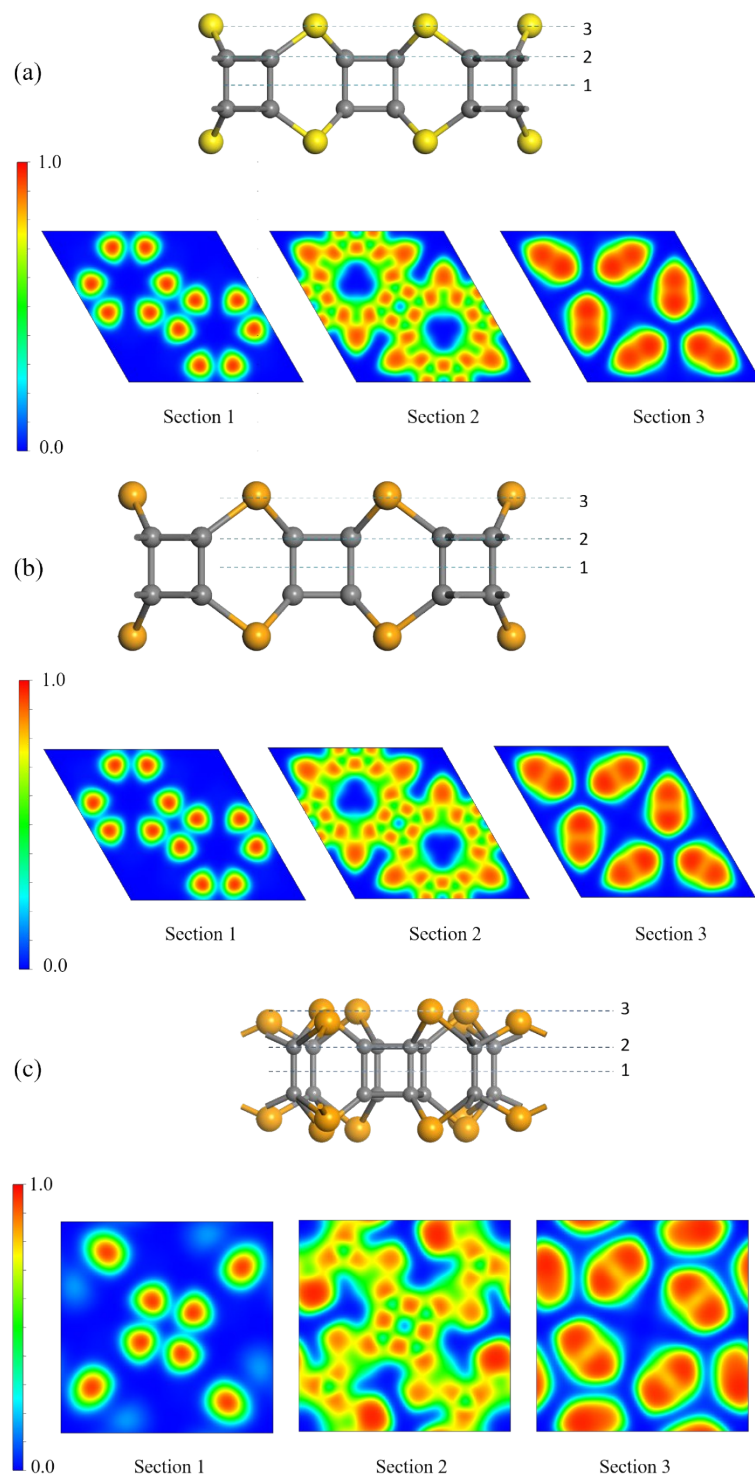


Fig. S2 ELF of (a) $C_{24}S_{12}$ (b) $C_{24}Se_{12}$ and (c) $C_{16}Se_{16}$

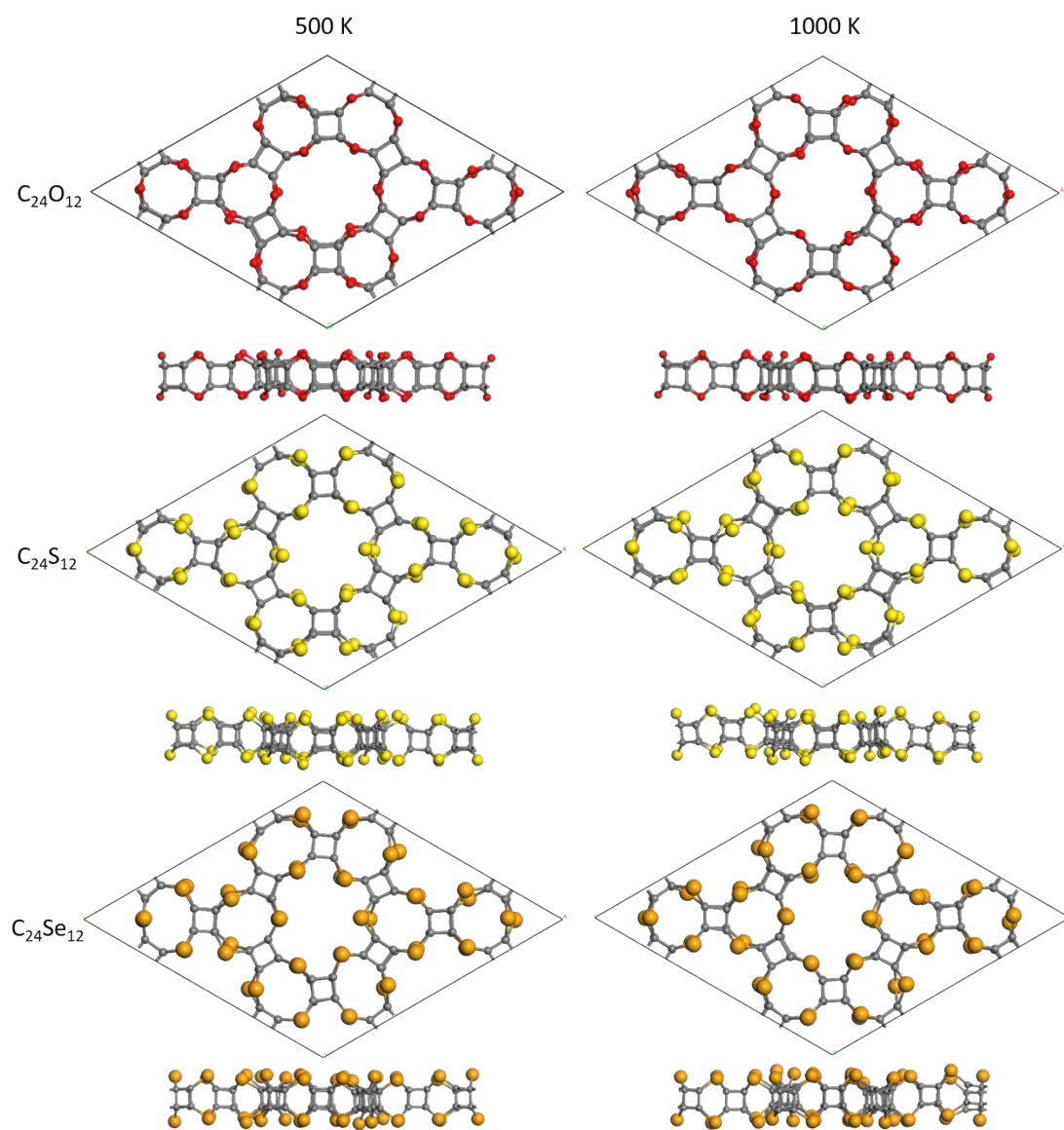
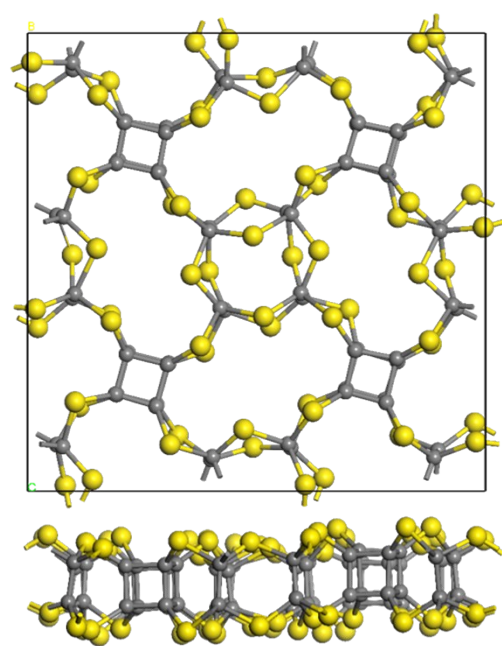
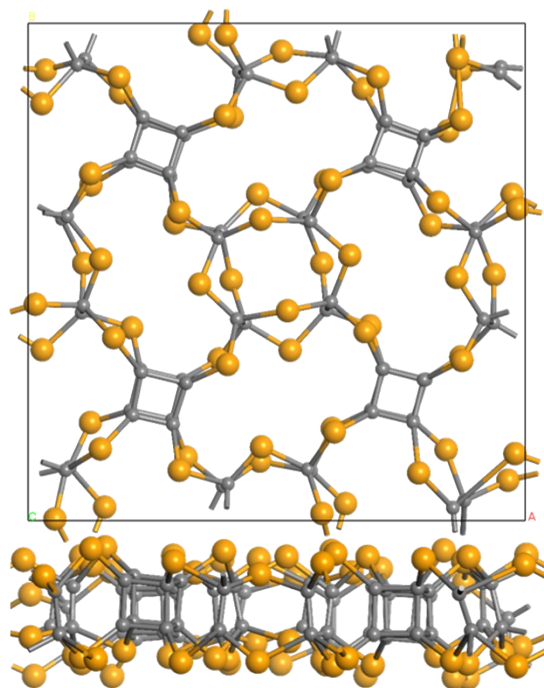


Fig. S3 Equilibrium configurations of $C_{24}X_{12}$ after 20 ps AIMD simulation under 500K and 1000K



$C_{16}S_{16}$



$C_{16}Se_{16}$

Fig. S4 Equilibrium configurations of $C_{16}X_{16}$ after 20 ps AIMD simulation under 500 K

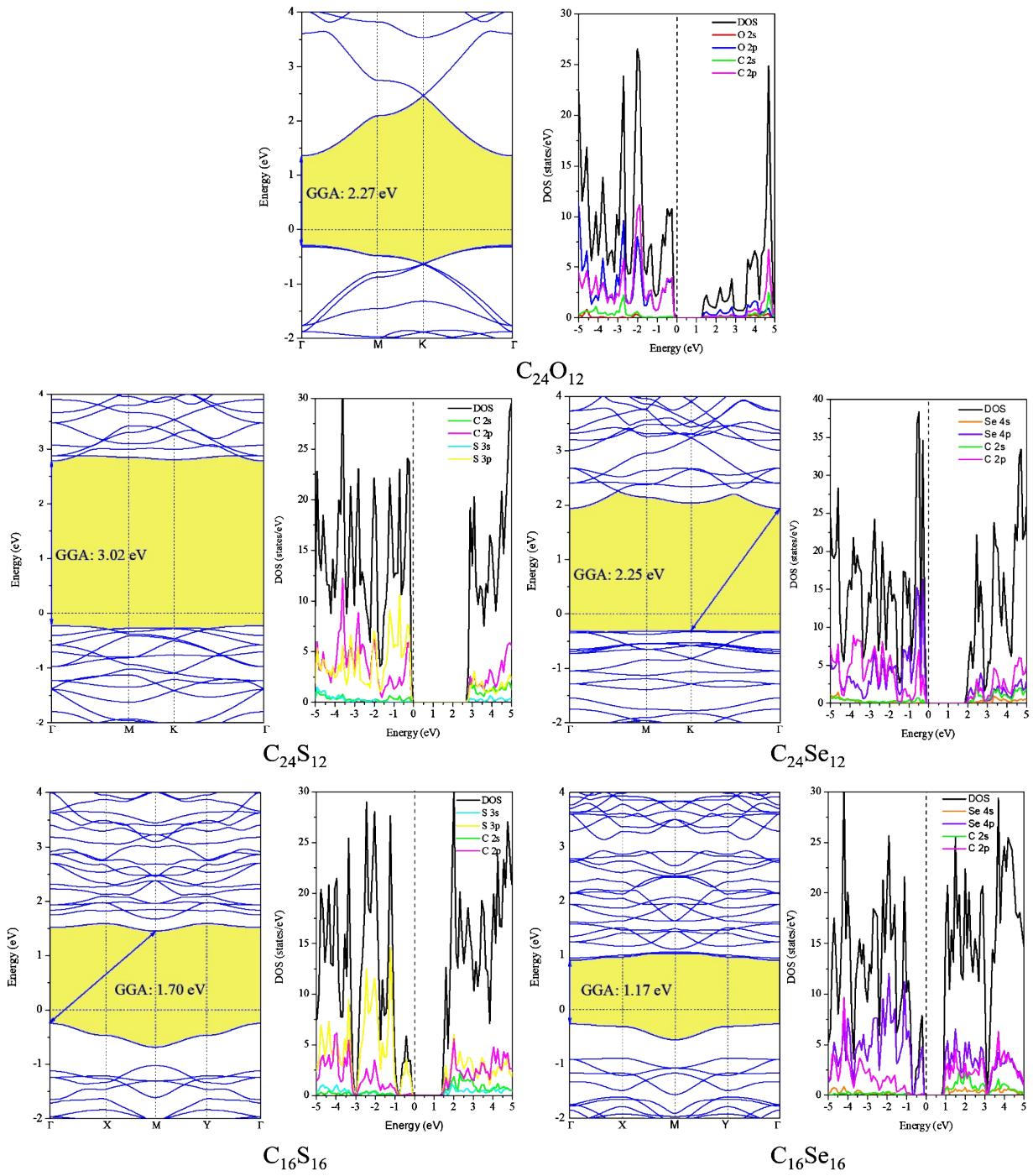


Fig. S5 Band structures and PDOS of $C_{24}X_{12}$ and $C_{16}X_{16}$ computed by GGA

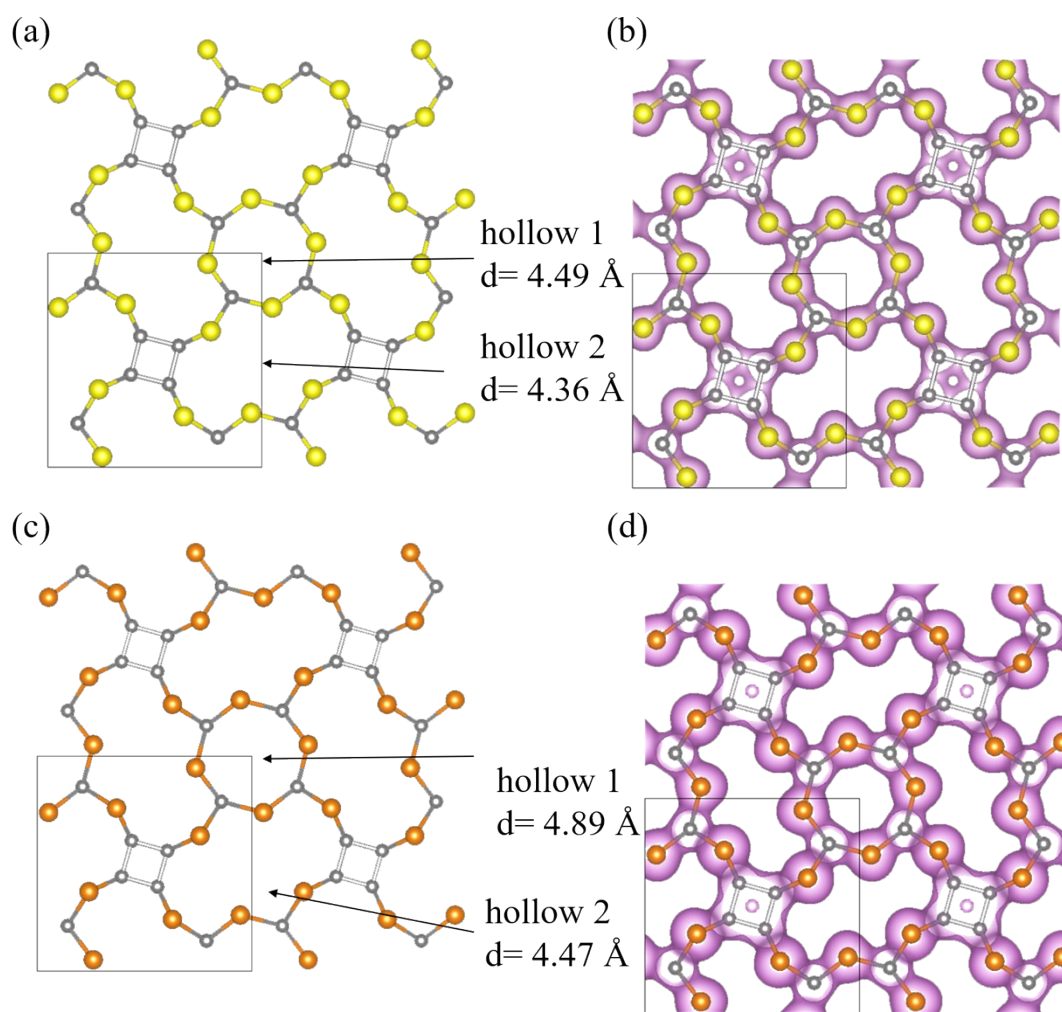


Fig. S6 Structures of (a) $C_{16}S_{16}$ and (c) $C_{16}Se_{16}$ and their corresponding electron densities, isovalue=0.05: (b) and (d)

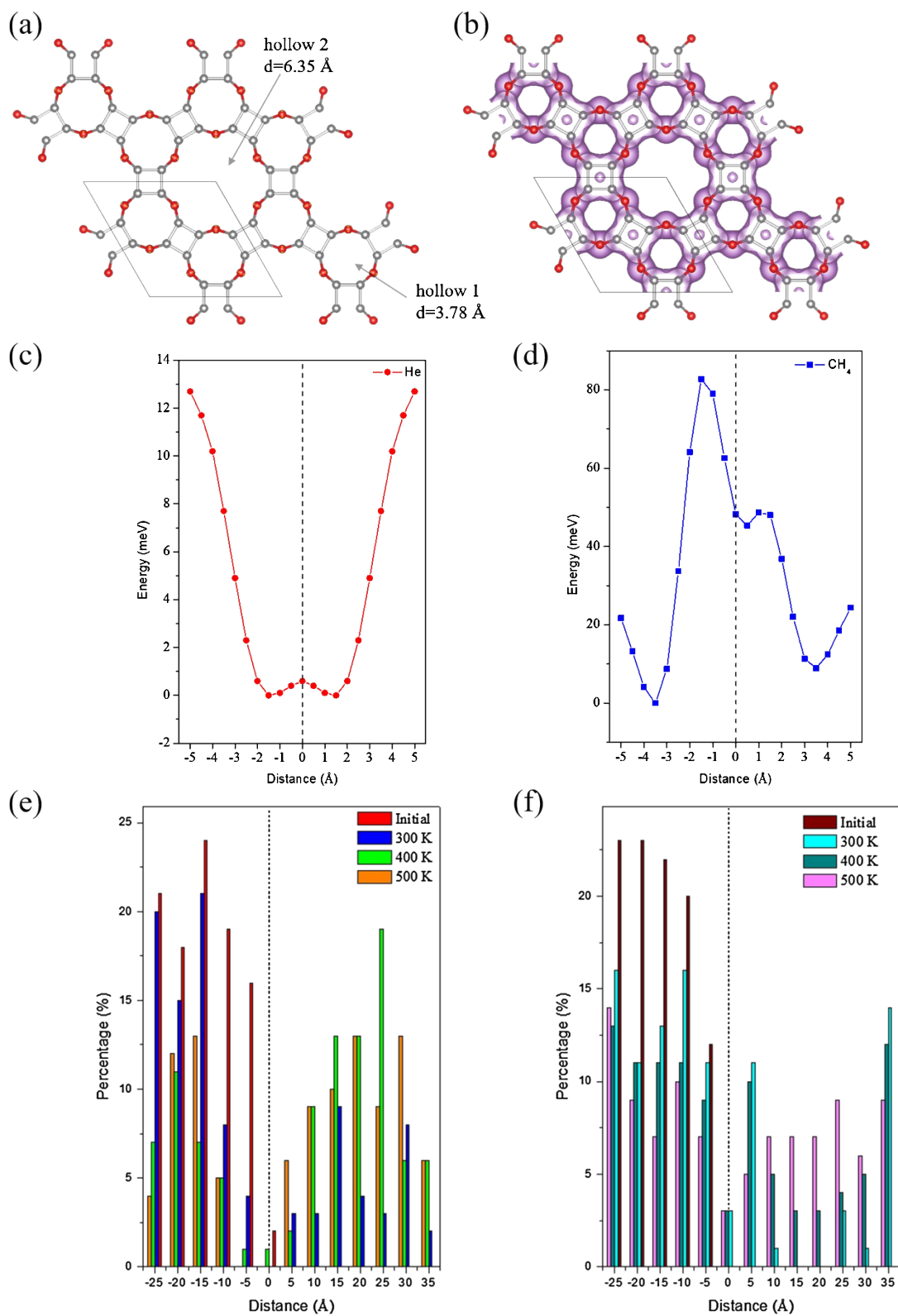


Fig. S7 (a) structure and (b) electron density of $C_{24}O_{12}$; energetic scan of (c) He and (d) methane pass through hollow 2; distribution of (e) He and (f) CH_4 after 2 ns MD simulations at 300, 400 and 500 K

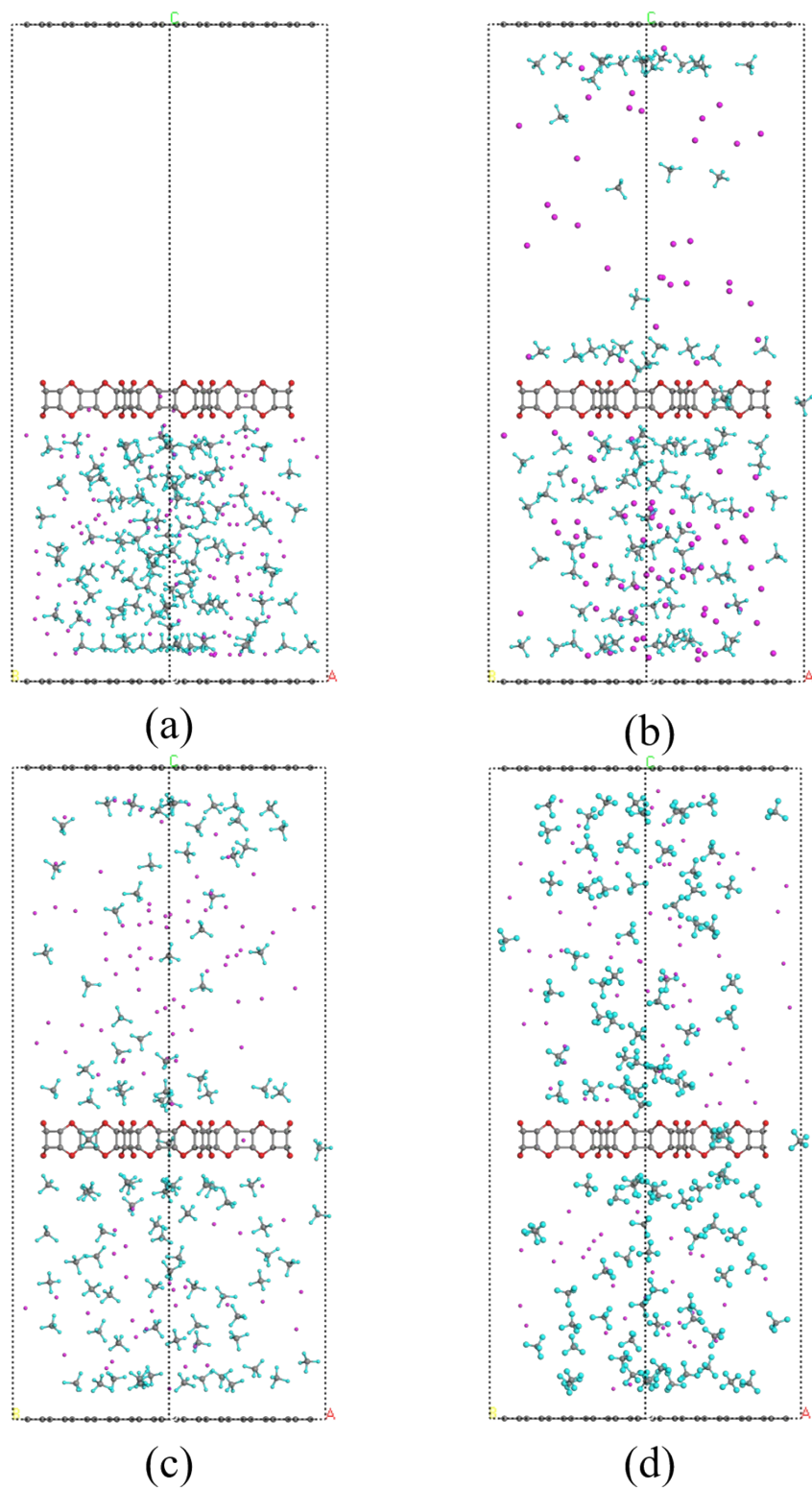


Fig. S8 (a) initial configuration and equilibrium structures after MD simulations under (b) 300 K, (c) 400 K and (d) 500 K of He/ CH_4 separation upon $C_{24}O_{12}$ monolayer. He atoms is colored in magenta.

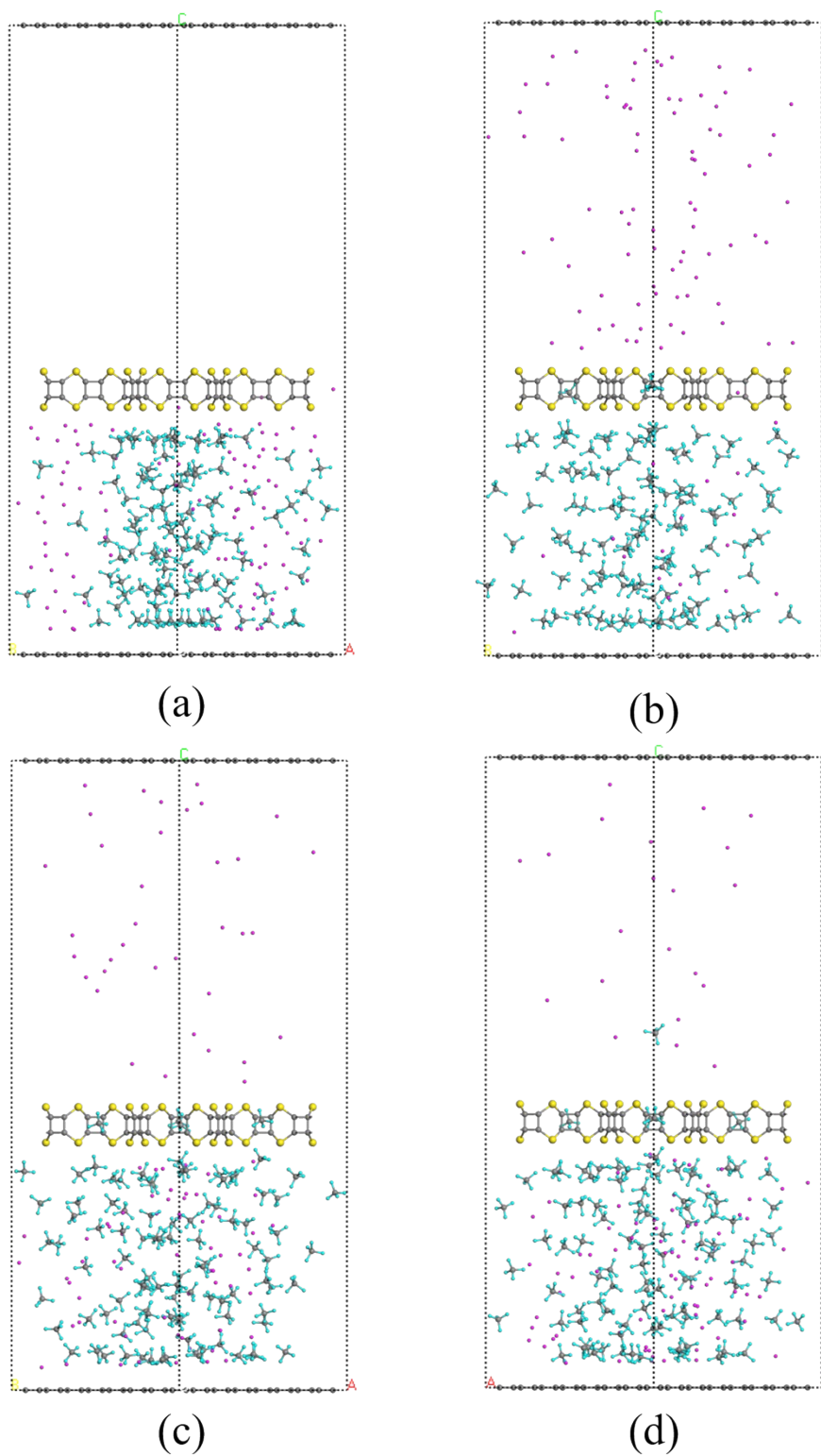


Fig. S9 (a) initial configuration and equilibrium structures after MD simulations under (b) 300 K, (c) 400 K and (d) 500 K of He/ CH_4 separation upon $C_{24}S_{12}$ monolayer

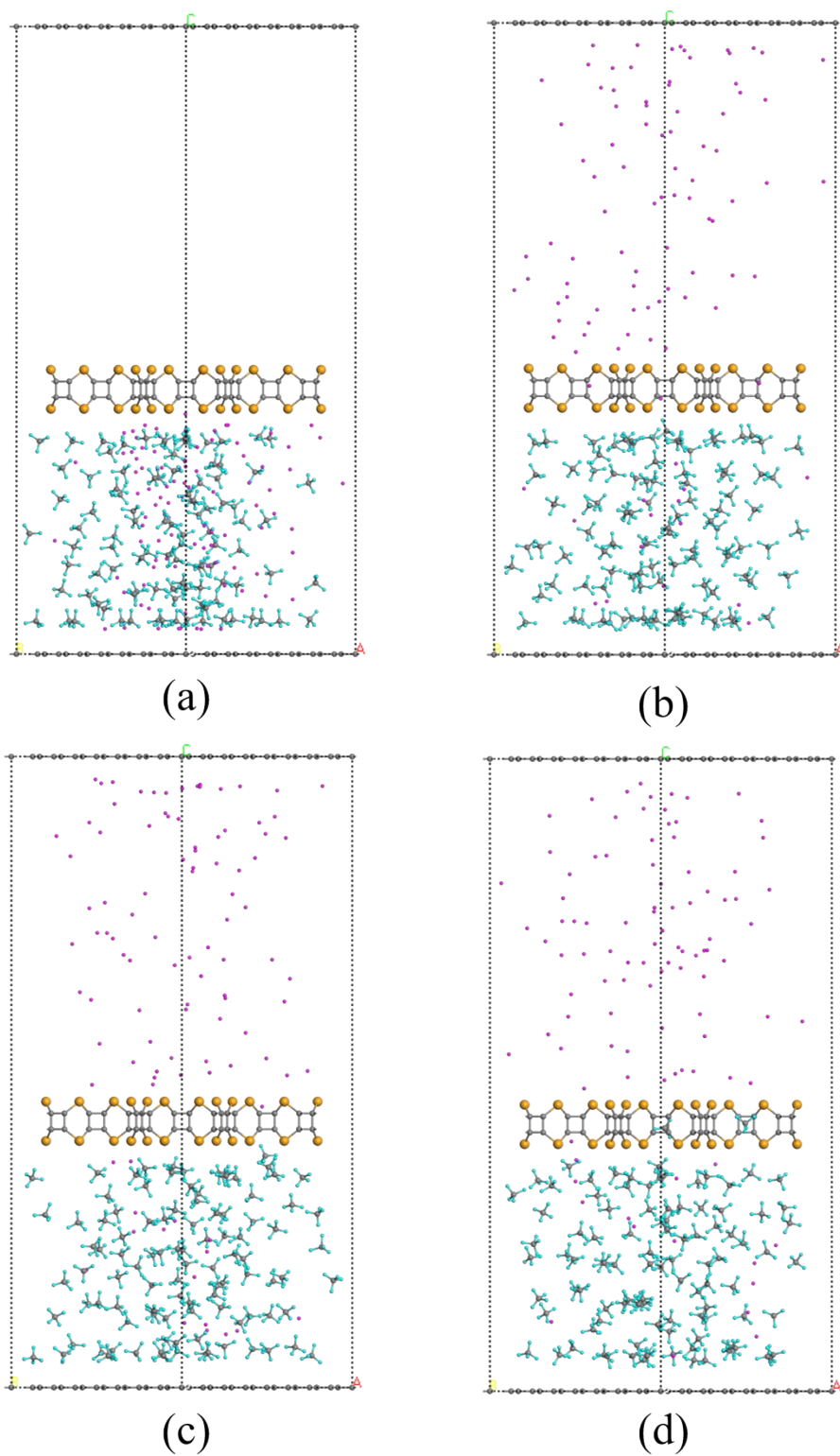


Fig. S10 (a) initial configuration and equilibrium structures after MD simulations under (b) 300 K, (c) 400 K and (d) 500 K of He/ CH_4 separation upon $C_{24}Se_{12}$ monolayer

Table S1 Length (Å) of C···S/Se and angle (°) of C-H···S/Se in CH₄@C₂₄S₁₂/ C₂₄Se₁₂ system

	Length	Angle
CH ₄ @C ₂₄ S ₁₂	2.87	167.7
	2.90	163.3
	3.06	141.4
	3.18	120.3
	3.05	163.7
CH ₄ @C ₂₄ Se ₁₂	3.08	157.0
	3.21	140.4
	3.33	122.7

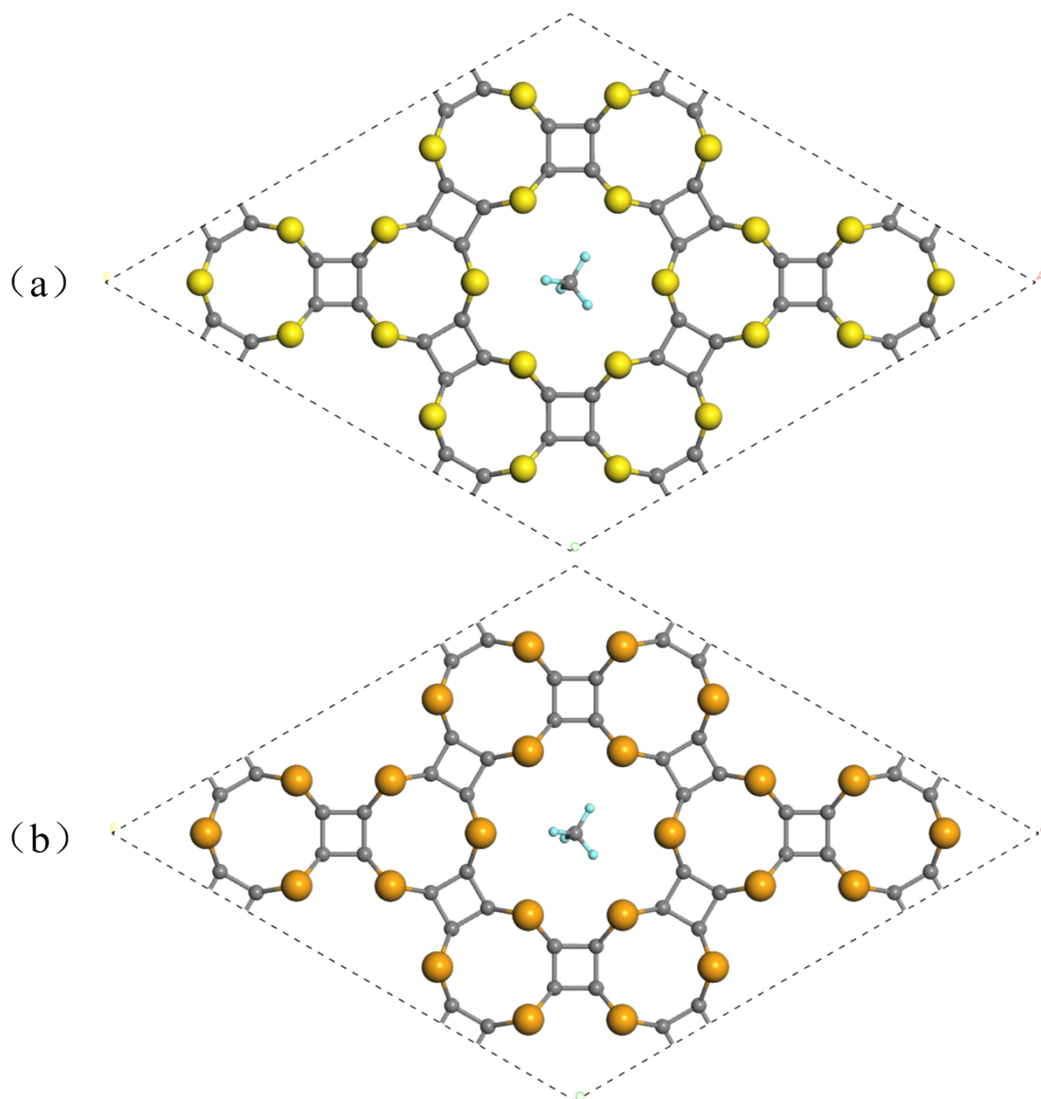


Fig. S11 Equilibrium structures of (a) CH₄@C₂₄S₁₂ and (b) CH₄@C₂₄Se₁₂