

Pt₇H₁₀(CH₃)@alpha₄rz Global Optimization Report

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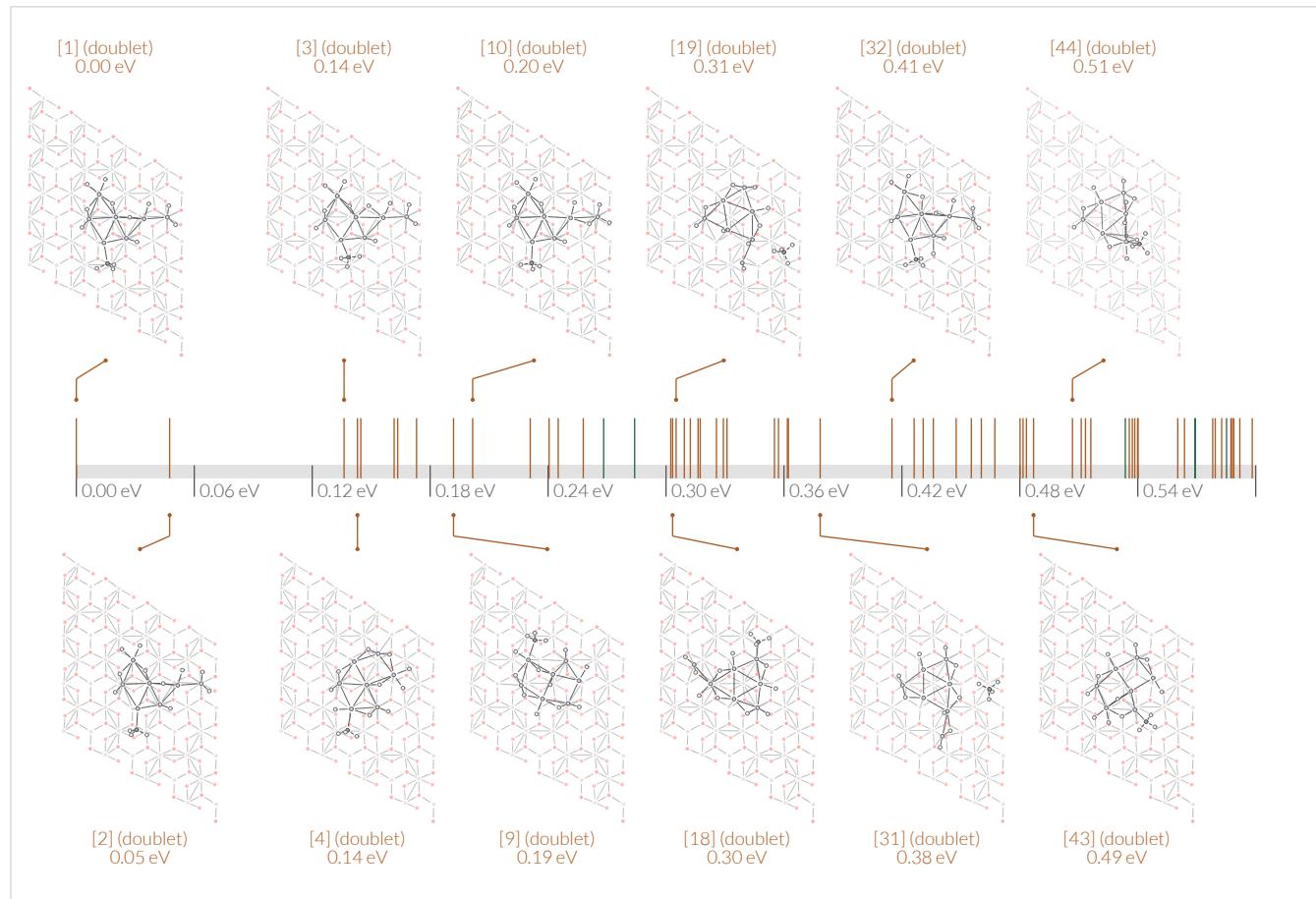
Energetics Summary

[Group I.A] Pt₇|H₁₀(CH₃)@alpha₄rz - blda - 10; VASP 5.4.1 :: PBE/

Multiplicity color: mixed, doublet. Element color: H, C, O, Al, Pt.

All energies are relative to the putative global minimum: -66.551041 [1] (#1.7.170), doublet.

Range: 0.00 ~ 0.60 eV (66 structures)



Command History

[I] final.zip

```
pgopt init "Pt7|H10(CH3)" 1 "--surface=alpha4rz" "--nodes=8"
pgopt set molecules+ CH3
pgopt set creation ~lowpos 0.1
pgopt set creation ~loworderelems H
pgopt set creation ~nomoleelems -CH3,H
pgopt set creation ~nocluselems -H,Al,H,O,C,-CH3,Al,H,O
pgopt set creation number 10
pgopt set mc
pgopt set mc temperature 1500
pgopt set mc short-distance-factor 0.85
pgopt set mc max-iter 300
pgopt set mc detailed-balance F
pgopt set mc swap-site T
pgopt set mc swap-site-make-space CH3
pgopt set mc swap-site-rate 0.25
pgopt set mc keep-ch3 T
pgopt set mc solid-move CH3
pgopt set mc light-shell T
pgopt set 0 relax
pgopt set 0 do-monte-carlo T
pgopt set 0 opts^
"sigma=0.1;encut=300;ediff=1E-4;ediffg=1E-3;lreal=A;scf(iter=300);lwave=F;algo=Fast;npar=16"
pgopt set 0 args step 50
pgopt set 0 args max_step 750
pgopt relax 1
pgopt transfer relax 1
pgopt torun para 0 10 "--time=12:00:00"
pgopt submit relax 1
pgopt submit torun para 0 10
pgopt submit relax 1
pgopt submit relax 1
# AFTER 13 HOURS
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt mclog
# AFTER 2 HOURS
```

```
pgopt mclog
# AFTER 27 HOURS
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 39 HOURS
pgopt log
pgopt set 0 args step 200
pgopt relax 1
pgopt transfer relax 1
pgopt torun para 0 10 "--time=12:00:00"
pgopt submit relax 1
pgopt submit torun para 0 10
# AFTER 26 HOURS
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
# AFTER 23 HOURS
pgopt log
pgopt mclog
# AFTER 24 HOURS
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
# AFTER 30 HOURS
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
```

```
pgopt submit torun para 0 10
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 13 HOURS
pgopt log
pgopt mclog
# AFTER 26 HOURS
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 7 HOURS
pgopt log
pgopt mclog
# AFTER 16 HOURS
pgopt log
pgopt mclog
# AFTER 23 HOURS
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt log
pgopt mclog
pgopt log
# AFTER 99 HOURS
pgopt log
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt mclog
pgopt mclog
# AFTER 23 HOURS
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 30 HOURS
pgopt log
```

```
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 15 HOURS
pgopt log
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 52 HOURS
pgopt log
pgopt mclog
pgopt submit relax 1
pgopt log
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10
pgopt depend torun para 0 10 --autodep
# AFTER 18 HOURS
pgopt log
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10
pgopt depend torun para 0 10 --autodep
# AFTER 5 HOURS
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 49 HOURS
pgopt log
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
```

```
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 1 HOURS
pgopt log
# AFTER 16 HOURS
pgopt log
pgopt mclog
pgopt mclog
# AFTER 24 HOURS
pgopt mclog
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
# AFTER 50 HOURS
pgopt log
pgopt mclog
pgopt mclog
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 23 HOURS
pgopt log
pgopt mclog
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
pgopt depend torun para 0 10 --autodep
pgopt submit torun para 0 10
# AFTER 18 HOURS
pgopt log
pgopt mclog
# AFTER 26 HOURS
pgopt log
```

```
pgopt mclog
pgopt log
pgopt mclog
# AFTER 3 HOURS
pgopt log
pgopt mclog
pgopt mclog
# AFTER 20 HOURS
pgopt log
pgopt mclog
pgopt torun para 0 5 "--time=12:00:00"
pgopt submit torun para 0 5
pgopt depend torun para 0 5 --autodep
pgopt submit torun para 0 5
pgopt depend torun para 0 5 --autodep
pgopt submit torun para 0 5
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
pgopt depend relax 1 --autodep
pgopt submit relax 1
# AFTER 22 HOURS
pgopt log
pgopt mclog
# AFTER 50 HOURS
pgopt log
pgopt mclog
# AFTER 389 HOURS
pgopt log
pgopt mclog
```

Global Information

	operating system	SUSE Linux Enterprise Server 12
	CPU	GenuineIntel @ 1200.203 MHz
	host name	onyx
	cores per node	44
	file name	final.zip
File I	total CPU hours	786668
	start	Oct 14, 2018 23:18:31
	finish	Nov 17, 2018 09:54:48
	times	33 days 11 hours 36 minutes 16 seconds
	running	16 days 15 hours 54 minutes 50 seconds
	idle	16 days 19 hours 41 minutes 26 seconds

Energy Computation Parameters

group id	program	basis	functional	charge	mini step	max step	disp step
I.A	VASP 5.4.1		PBE	0	200	750	0.0

Local Optimization Options

I.A-1.0.0 (relax*): scf(iter=300);cell=16.6533:-9.6148:0.0000:19.2296:25.6679;fix(0-143);nocenter;encut=300;algo=Fast;ediffg=1E-3;ediff=1E-4;lwave=F;npar=16;sigma=0.1;lreal=A

Creation Parameters

	name	Pt ₇ H ₁₀ (CH ₃)@alpha ₄ rz
	method	BLDA (Bond Length Distribution Algorithm)
	number	10
	order	2
I.A.1	C-C	[1] 1.540 Å± 0.100 [2] 1.540 Å± 0.400
	C-H	[1] 1.140 Å± 0.100 [2] 1.140 Å± 0.400
	H-H	[1] 0.740 Å± 0.100 [2] 0.740 Å± 0.400
	Pt-C	[1] 2.050 Å± 0.100 [2] 2.050 Å± 0.400
	Pt-H	[1] 1.650 Å± 0.100 [2] 1.650 Å± 0.400
	Pt-Pt	[1] 2.560 Å± 0.100 [2] 2.560 Å± 0.400

Filtering Parameters

group id	creation		runtime		final	
	max diff	report	max diff	report	max diff	report
I.A	0.25	1.00	0.10	0.15	0.25	1.00

Job Parallelism Information

group id	run id	task	average available processors	average running processors	maximum available processors	maximum running processors	cores per processors
I.A	1.0.0	relax	3	3	10	10	352

Job Time Information

group id	run id	task	total wall time	total node hours	total CPU hours	total cost CPU hours
I.A	1.0.0	relax	803:36:20	2848	786668	1002568

Primary Configurations

group id	run id	sources	total	failed	max	converged	minima	transition states	duplicates
I.A	1.0.0	create	10	0	0	10	0	0	0

Primary Times

group id	run id	sources	total	failed	converged	minima	transition states	duplicates
I.A	1.0.0	create	786436	0	786436	0	0	0

Filtered Configurations

group id	multiplicity	minima	transition states	unknowns	filtered minima	filtered transition states	filtered unknowns
I.A	mixed	0	0	2860	0	0	2607

Optimization Time and Steps

group id	run id	task	sources	number	steps			time		
					mean	max	min	mean	max	min
I.A	1.0.0	relax	create	10	171	548	30	44:42	6:44:14	9:41

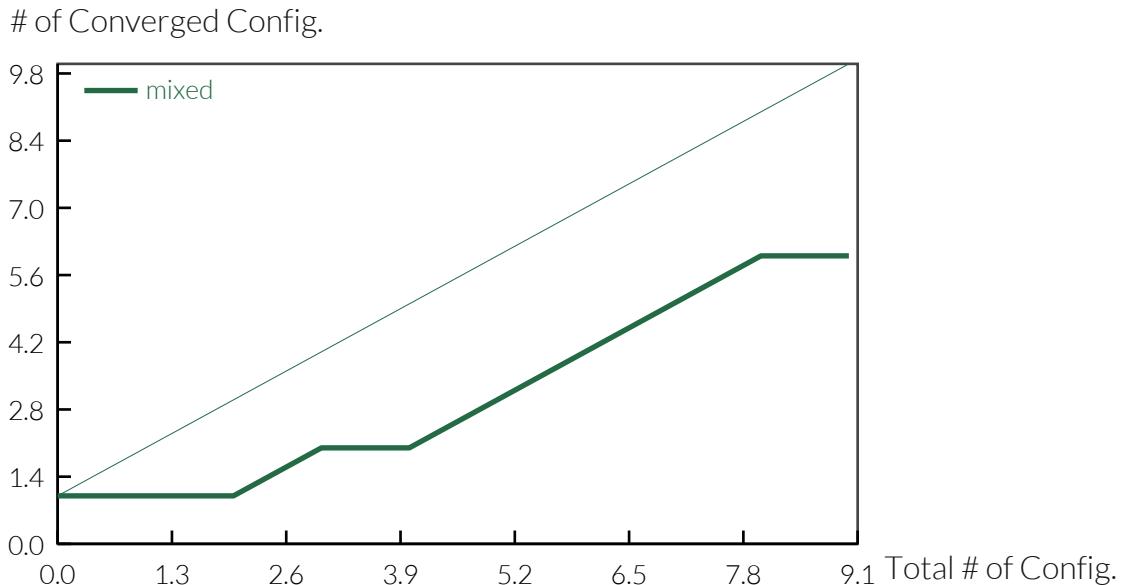
Energetics

stage	run id	sources	minimum	delta (eV)	maximum	delta (eV)
I.A initial	1.0.0	create	-66.303397	6.739	-63.890501	72.397
I.A final	1.0.0	create	-66.551041	0.000	-66.089335	12.564

Configuration Convergence

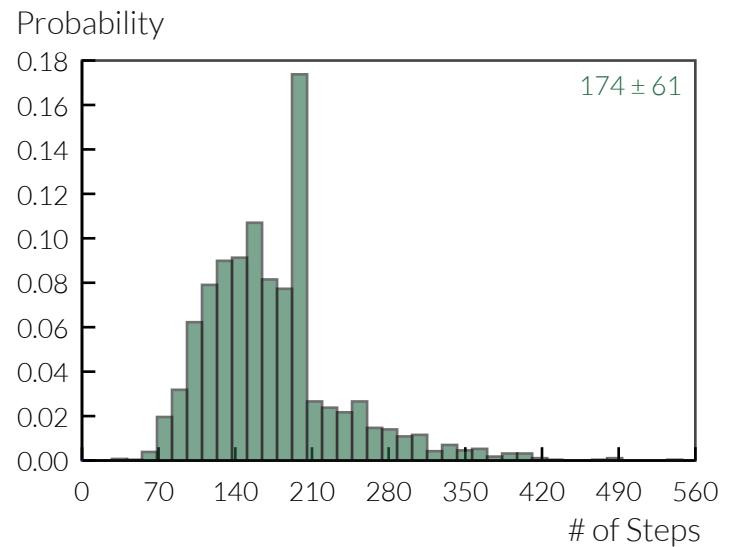
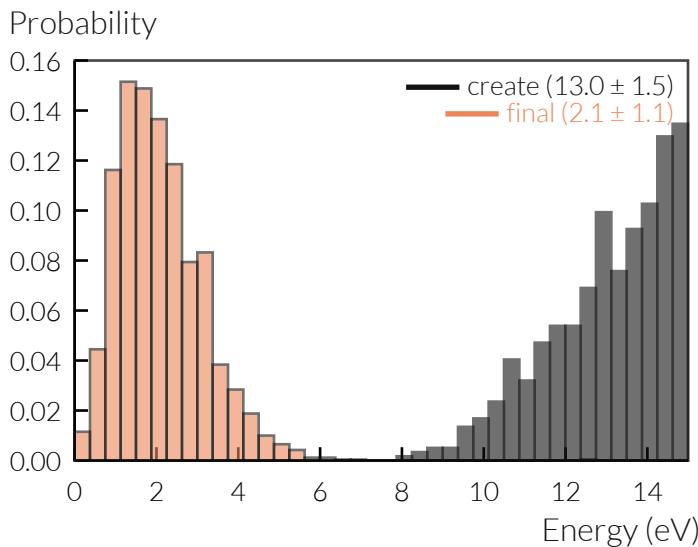
Thick lines: converged structures with energy up to 0.40 eV with respect to global minimum of each multiplicity.
Thin lines: all converged structures.

[Stage I.A.1] Pt₇|H₁₀(CH₃)@alpha₄rz - blda - 10; VASP 5.4.1 :: PBE/



Energy and Step Distribution

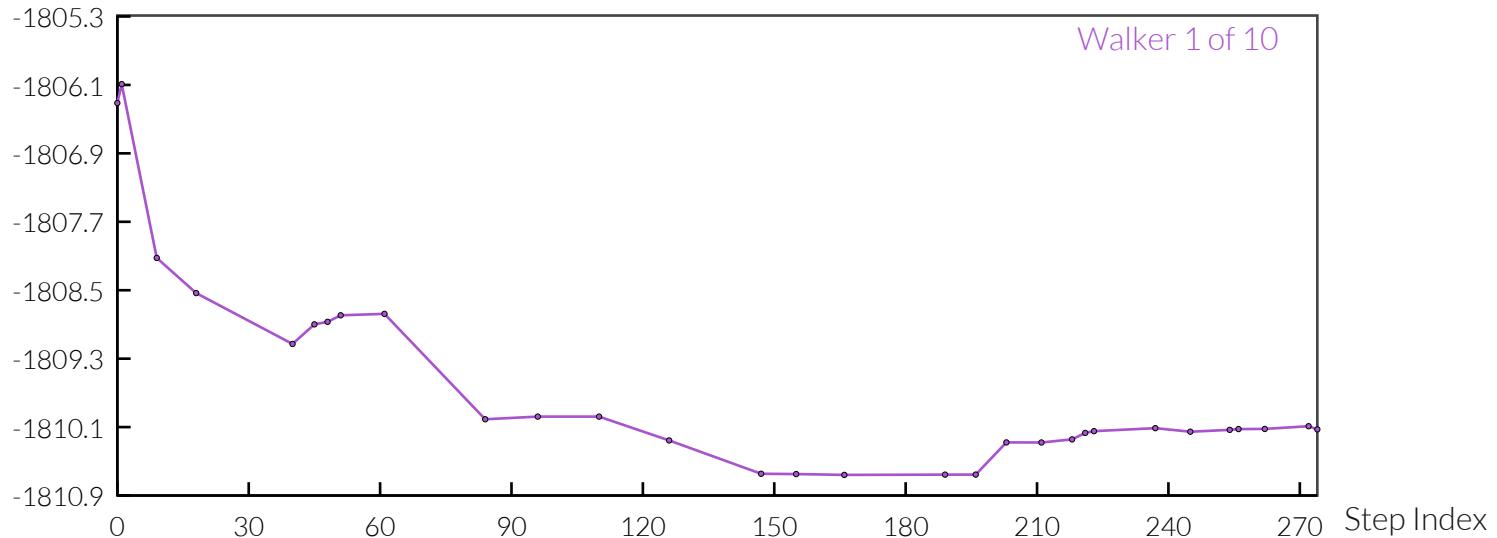
[Group I.A] Pt₇|H₁₀(CH₃)@alpha₄rz - blda - 10; VASP 5.4.1 :: PBE/



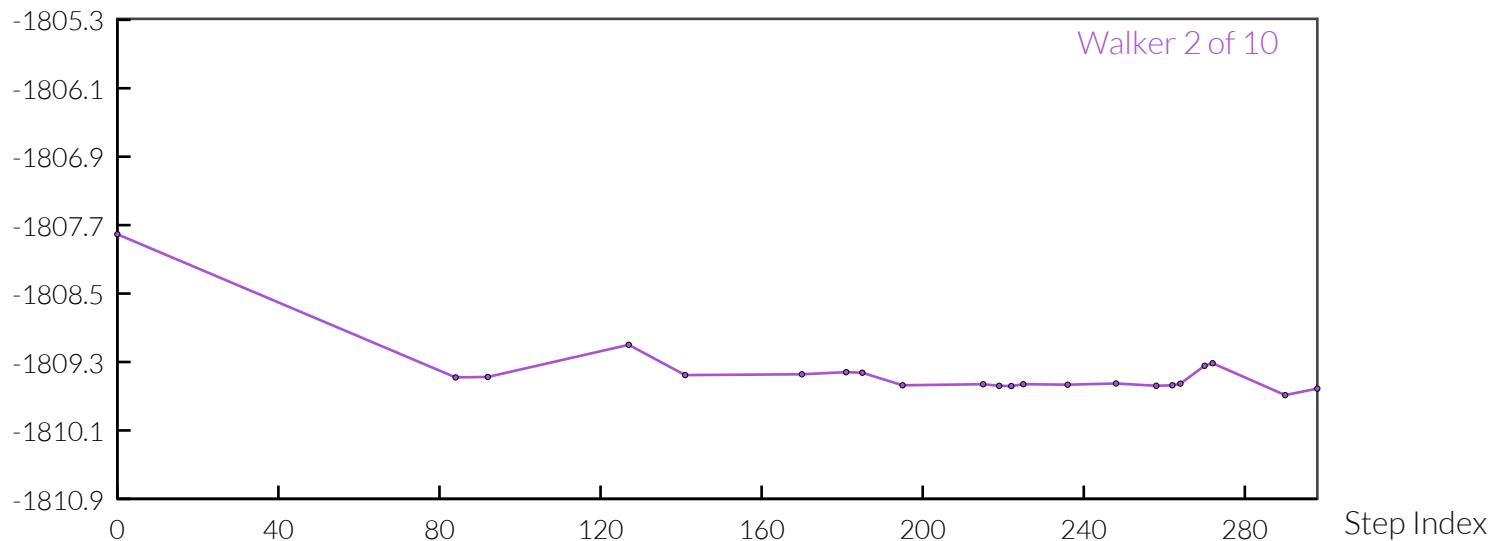
Monte-Carlo Energetics

[Run I.A.1 (M=0)] Pt₇|H₁₀(CH₃)@alpha₄rz - blda - 10; VASP 5.4.1 :: PBE/

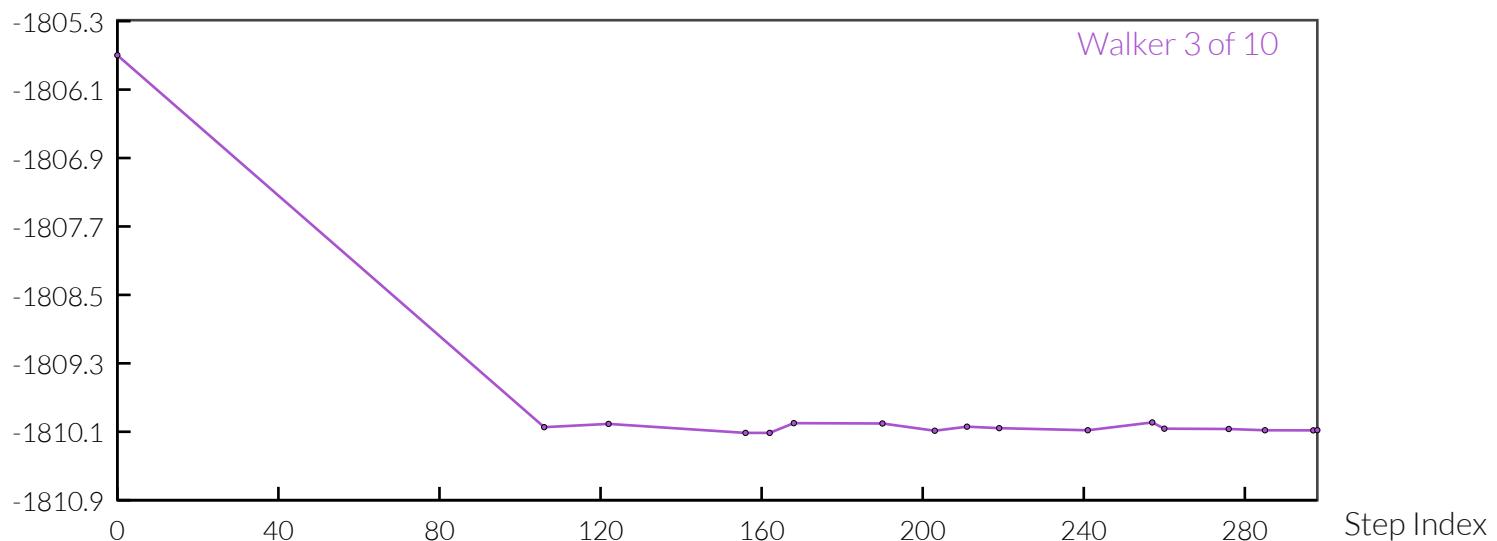
Accepted Relaxed Energy (eV)



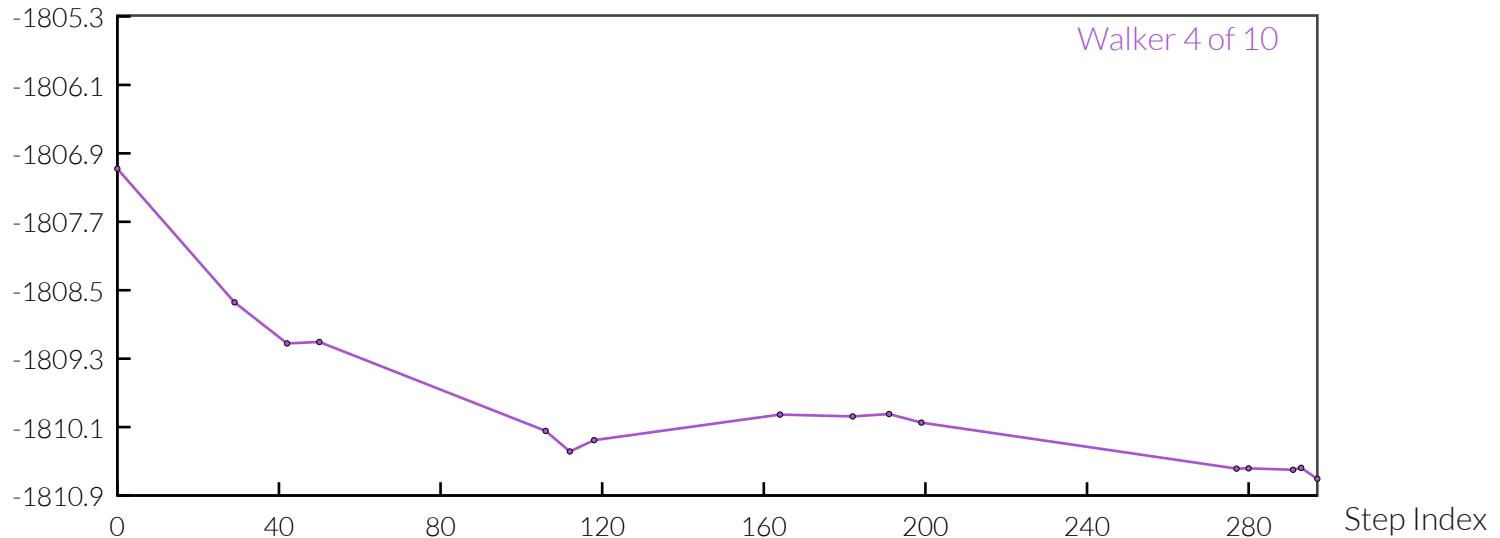
Accepted Relaxed Energy (eV)



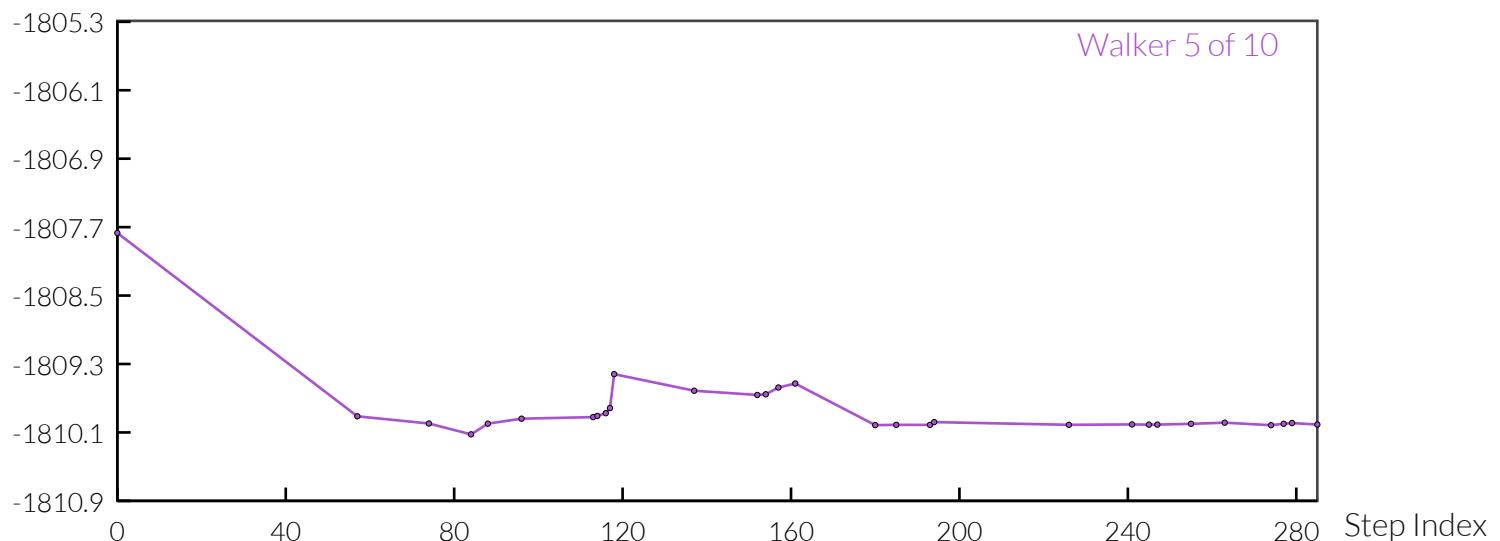
Accepted Relaxed Energy (eV)



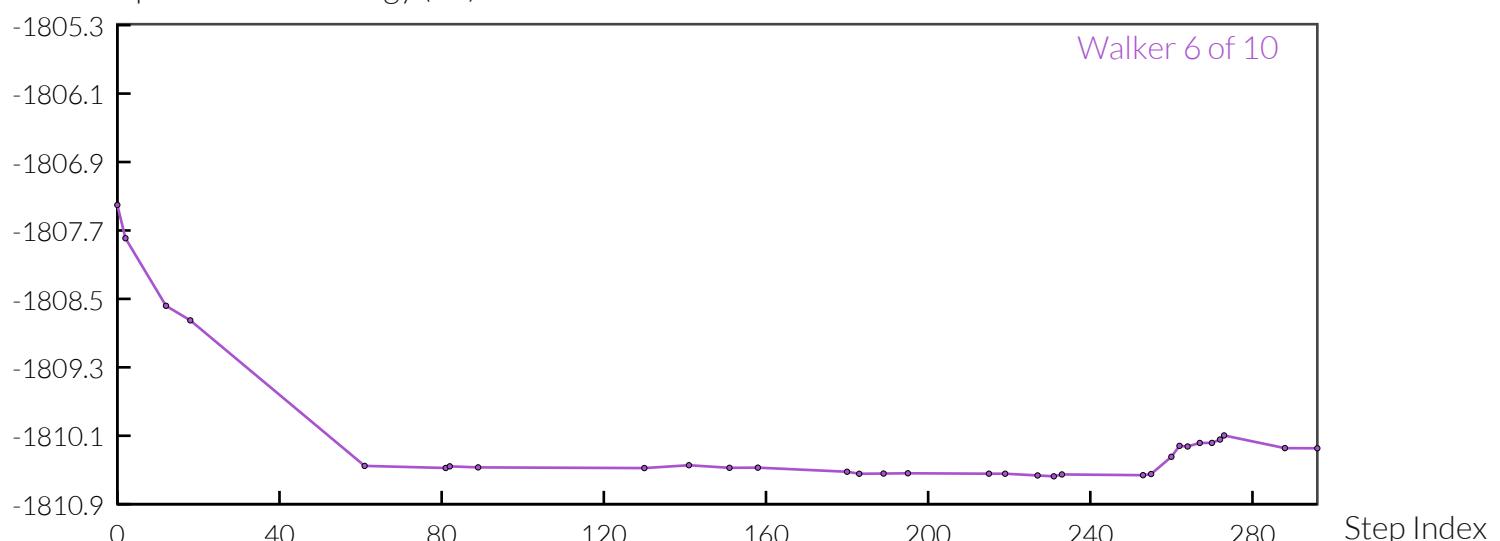
Accepted Relaxed Energy (eV)



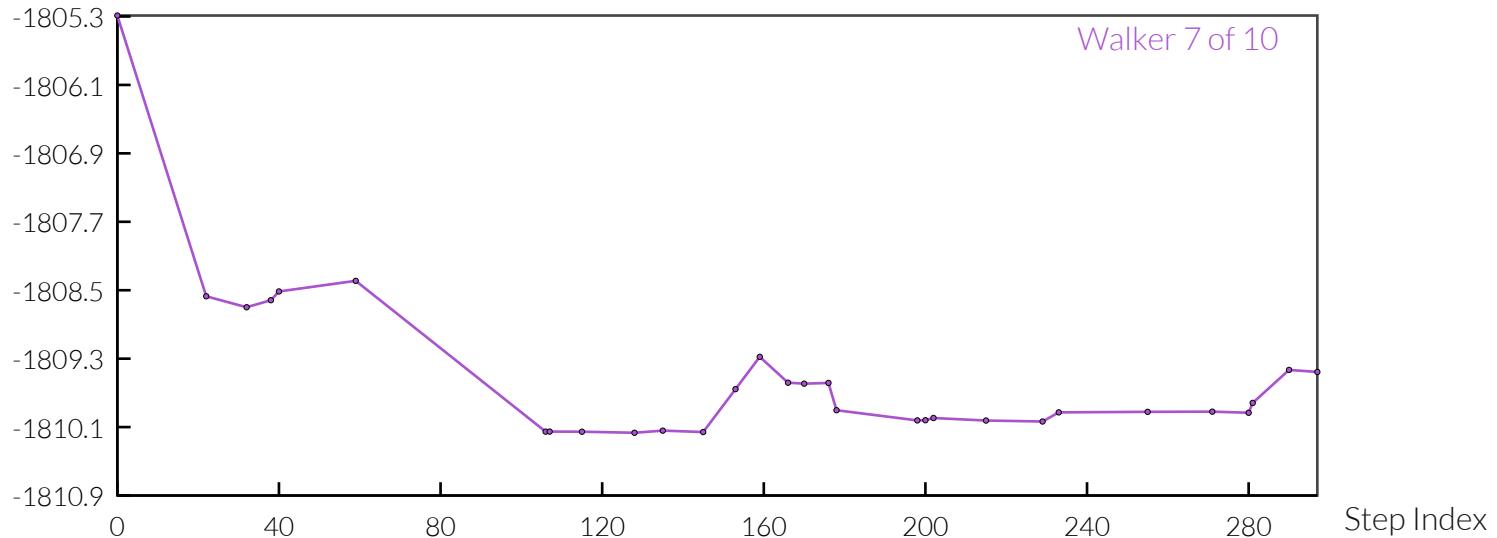
Accepted Relaxed Energy (eV)



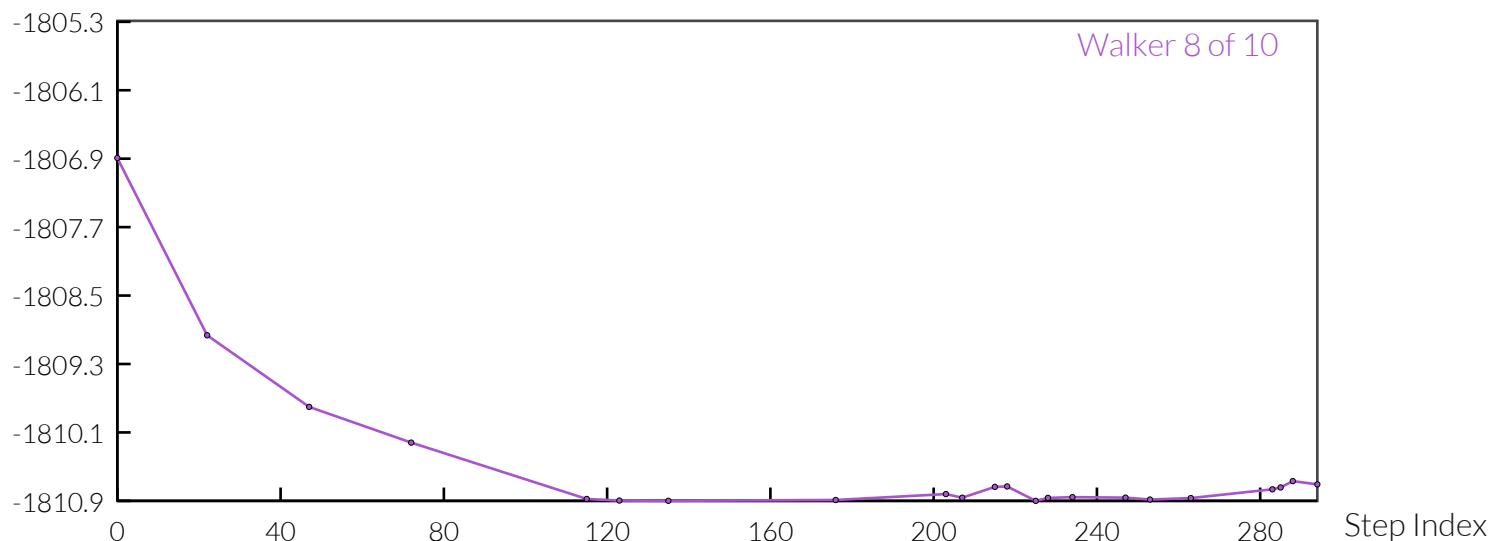
Accepted Relaxed Energy (eV)



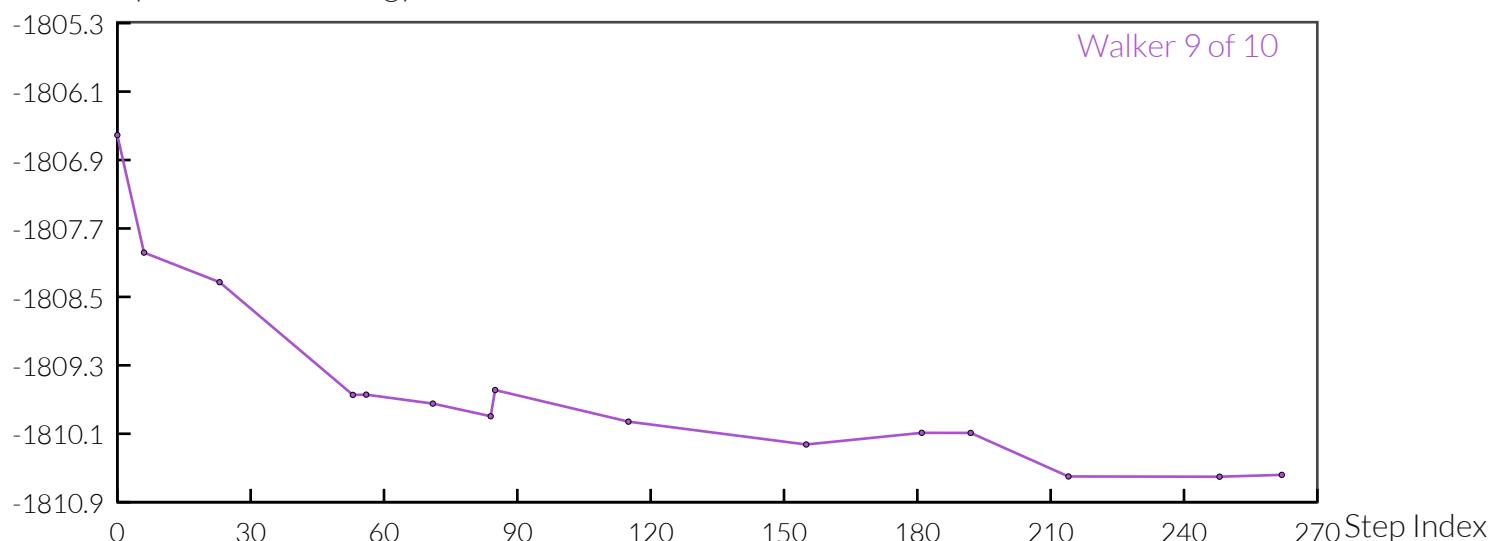
Accepted Relaxed Energy (eV)



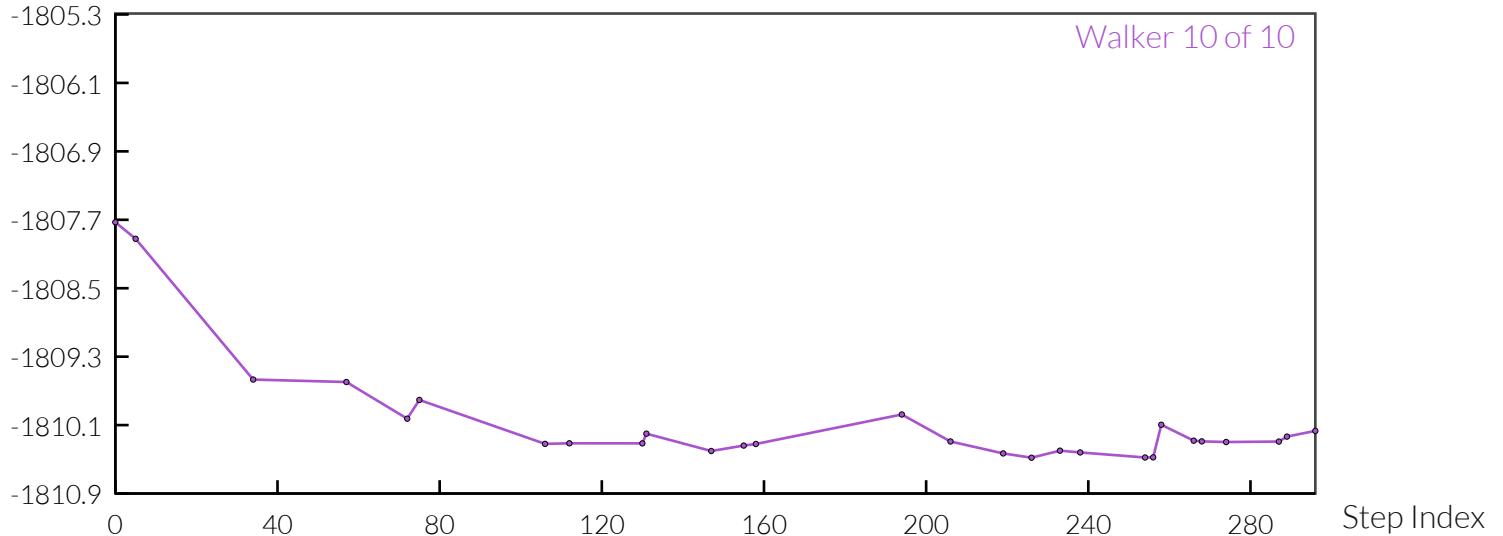
Accepted Relaxed Energy (eV)



Accepted Relaxed Energy (eV)



Accepted Relaxed Energy (eV)



Boltzmann Distribution Probabilities

[Group I.A] Pt₇|H₁₀(CH₃)@alpha₄rz - blda - 10; VASP 5.4.1 :: PBE/

name	multiplicity	E (eV)	P (100K)	P (300K)	P (400K)	P (500K)	P (700K)	P (1000K)
[1] #1.7.170 * 30	doublet	0.00000	0.49899	0.93917	0.84842	0.64379	0.46273	0.28518
[2] #1.7.247	doublet	0.04746	0.00000	0.05982	0.13532	0.21399	0.21069	0.16441
[3] #1.7.284 * 2	doublet	0.13621		0.00035	0.00437	0.02728	0.04838	0.05870
[4] #1.3.153 * 4	doublet	0.14302		0.00023	0.00336	0.02329	0.04321	0.05424
[5] #1.7.283	doublet	0.14473		0.00021	0.00314	0.02238	0.04201	0.05317
[6] #1.8.286 * 3	doublet	0.16168		0.00008	0.00163	0.01510	0.03172	0.04368
[7] #1.8.296	doublet	0.16348		0.00007	0.00152	0.01448	0.03078	0.04278
[8] #1.7.215 * 3	doublet	0.17309		0.00004	0.00105	0.01159	0.02625	0.03826
[9] #1.3.299 * 4	doublet	0.19189		0.00001	0.00051	0.00749	0.01922	0.03076
[10] #1.7.292 * 3	doublet	0.20164		0.00035	0.00597	0.01635	0.02747	
total (10 of 2607)	(* 52 of 2998)		0.50101	1.00000	0.99966	0.98536	0.93134	0.79866

Details

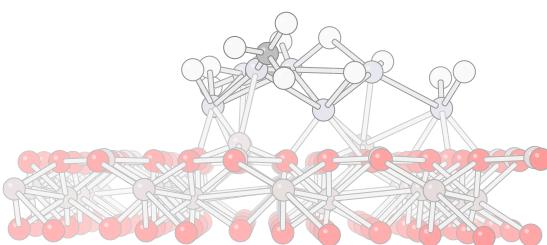
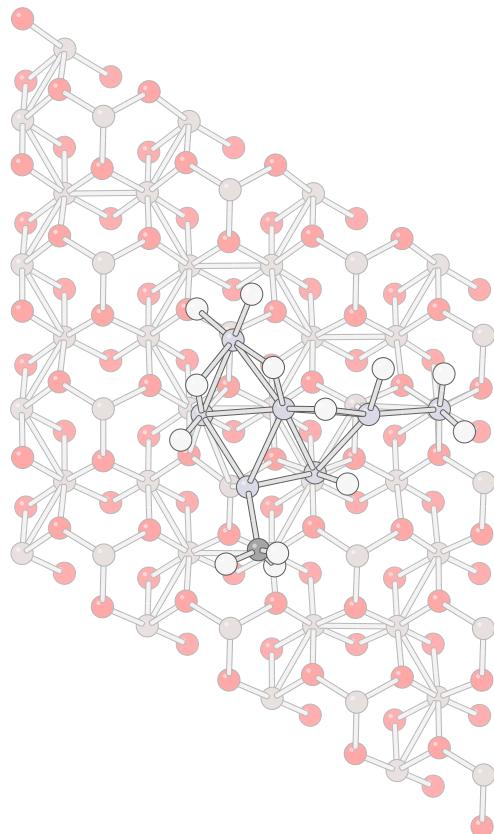
Note: Only structures with energy up to 0.60 eV with respect to global minimum are listed.

[Group I.A] Pt₇|H₁₀(CH₃)@alpha₄rz - blda - 10; VASP 5.4.1 :: PBE/

[1] #1.7.170 UNK (doublet)

E = -66.551041 (0.000 eV)

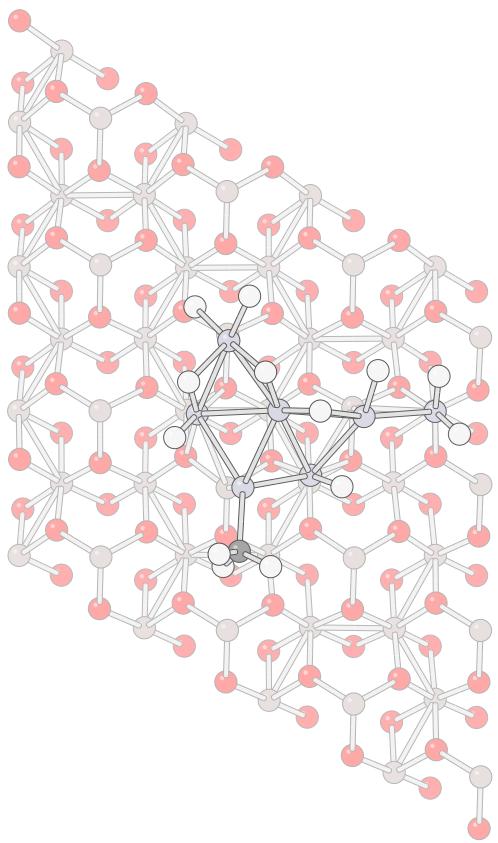
[Relax] Time: 23:37 Step: 102



[2] ~ [1] (d = 0.26) #1.7.247 UNK (doublet)

E = -66.549297 (0.047 eV)

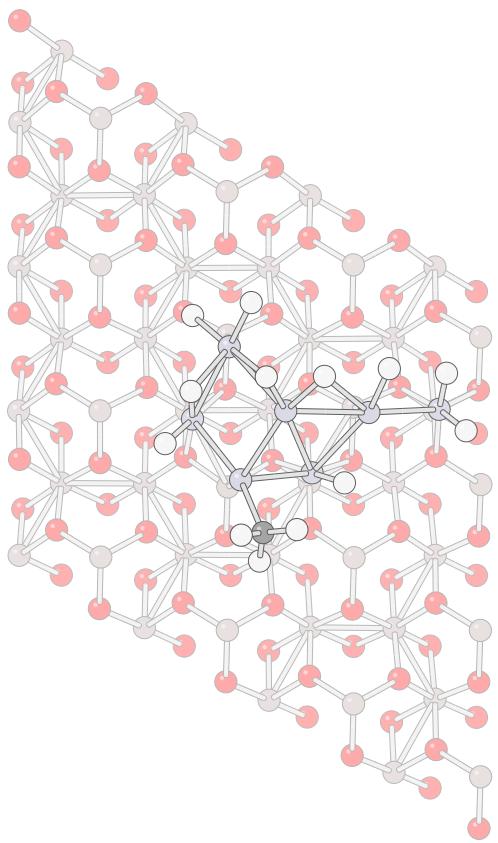
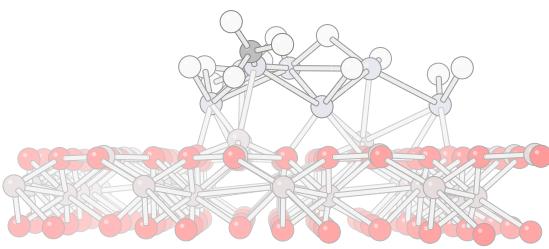
[Relax] Time: 24:05 Step: 106



[3] ~ [1] (d = 0.45) #1.7.284 UNK (doublet)

E = -66.546035 (0.136 eV)

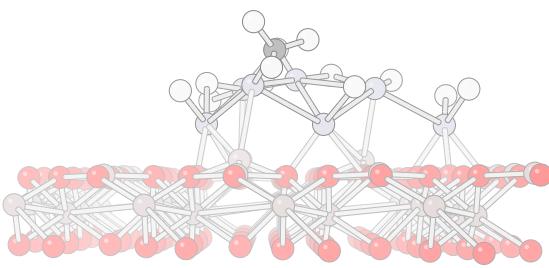
[Relax] Time: 27:53 Step: 135

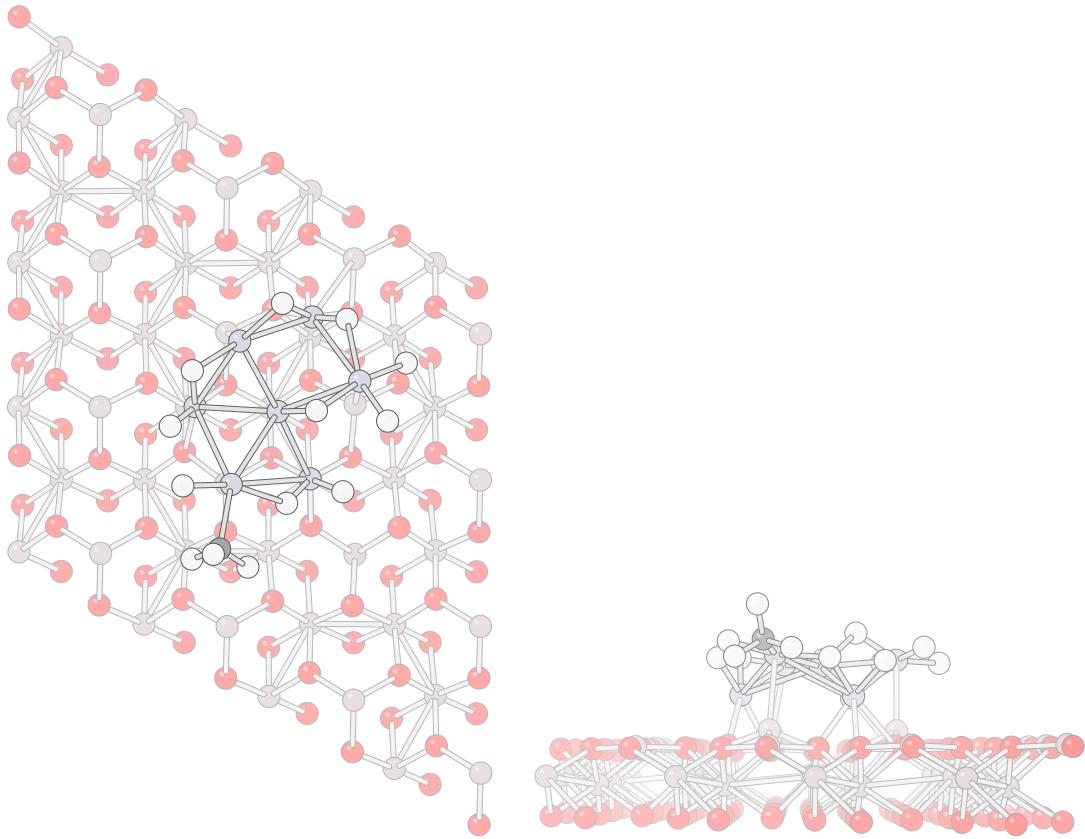


[4] ~ [2] (d = 1.29) #1.3.153 UNK (doublet)

E = -66.545785 (0.143 eV)

[Relax] Time: 22:59 Step: 97

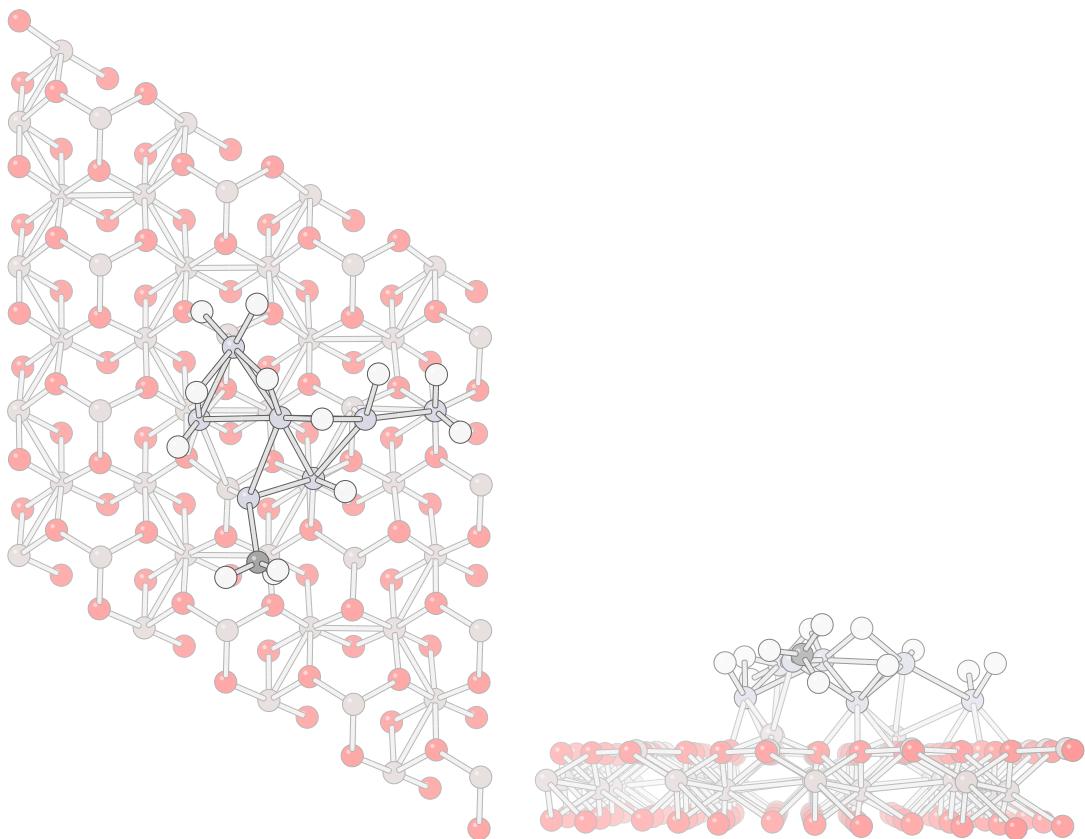




[5] ~ [1] ($d = 0.26$) #1.7.283 UNK (doublet)

$E = -66.545722$ (0.145 eV)

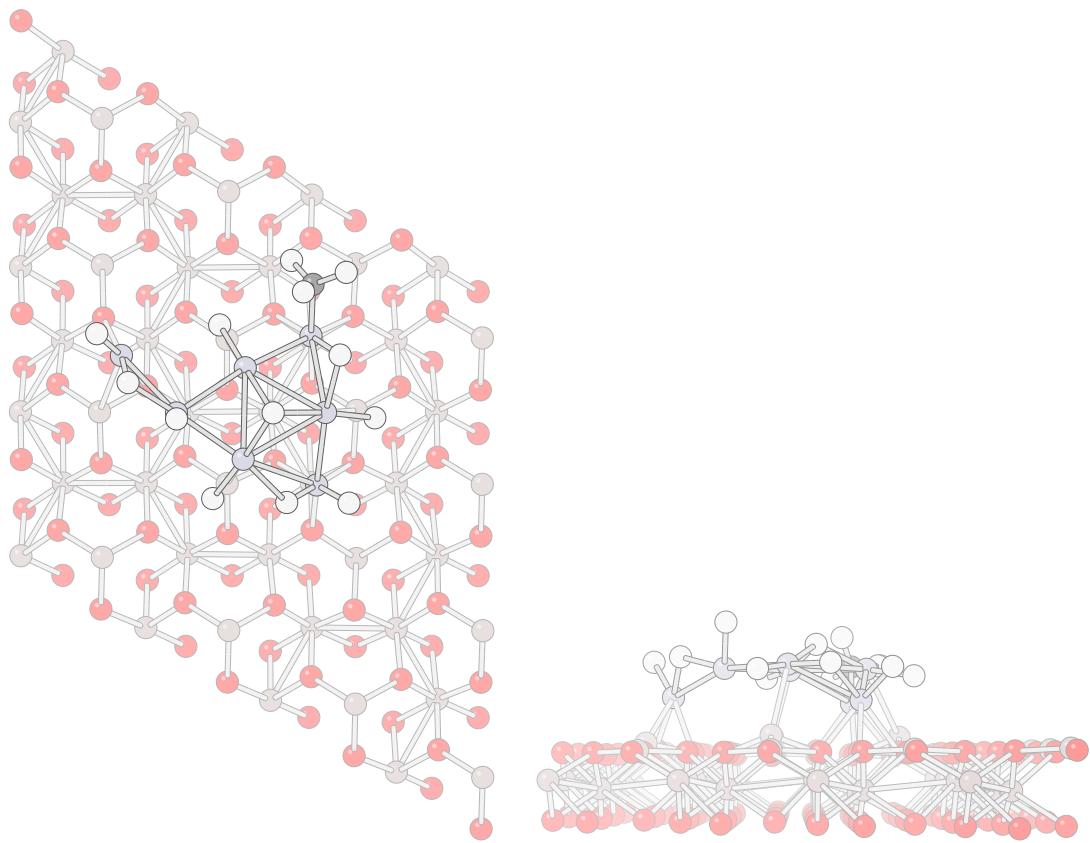
[Relax] Time: 13:50 Step: 41



[6] ~ [4] ($d = 1.69$) #1.8.286 UNK (doublet)

$E = -66.545099$ (0.162 eV)

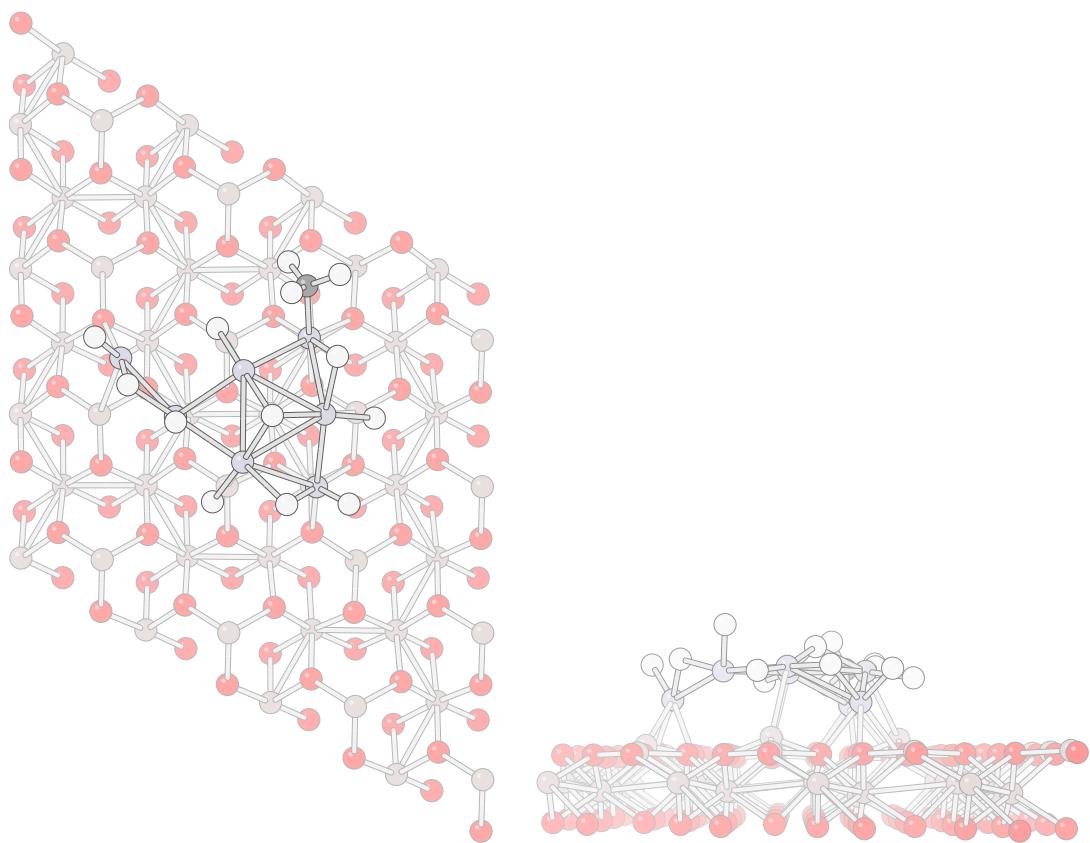
[Relax] Time: 34:29 Step: 110



[7] ~ [6] (d = 0.37) #1.8.296 UNK (doublet)

E = -66.545033 (0.163 eV)

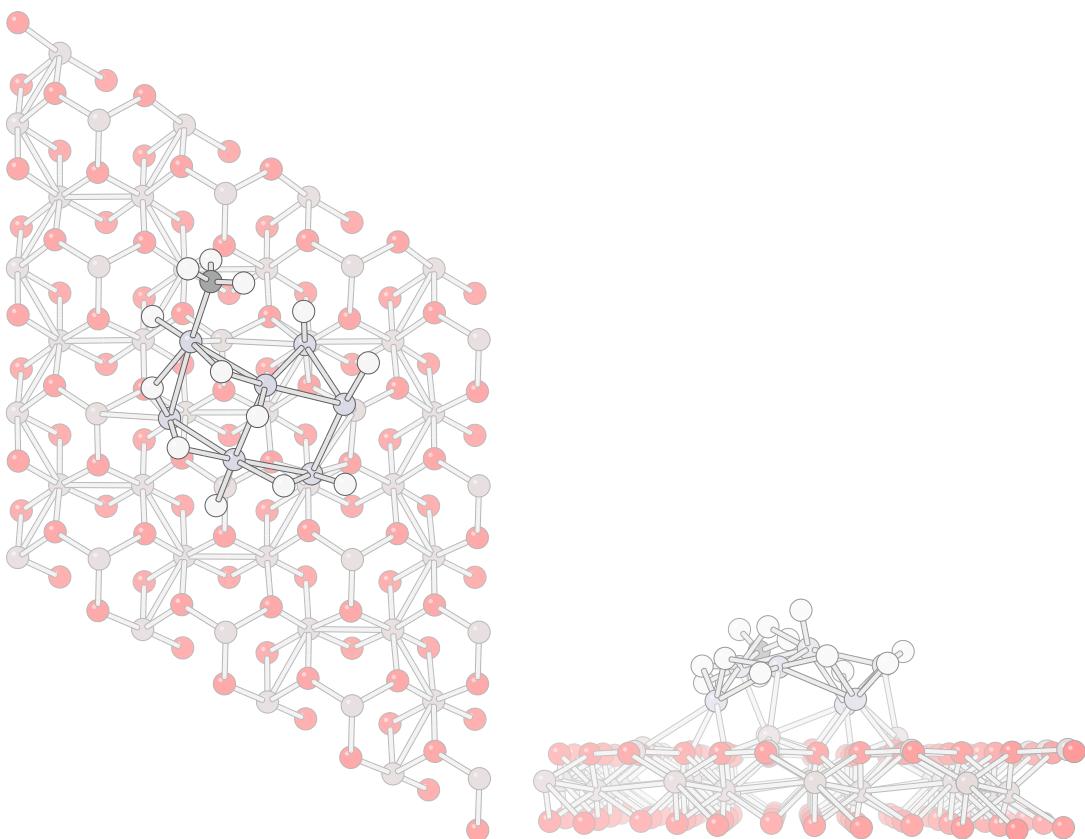
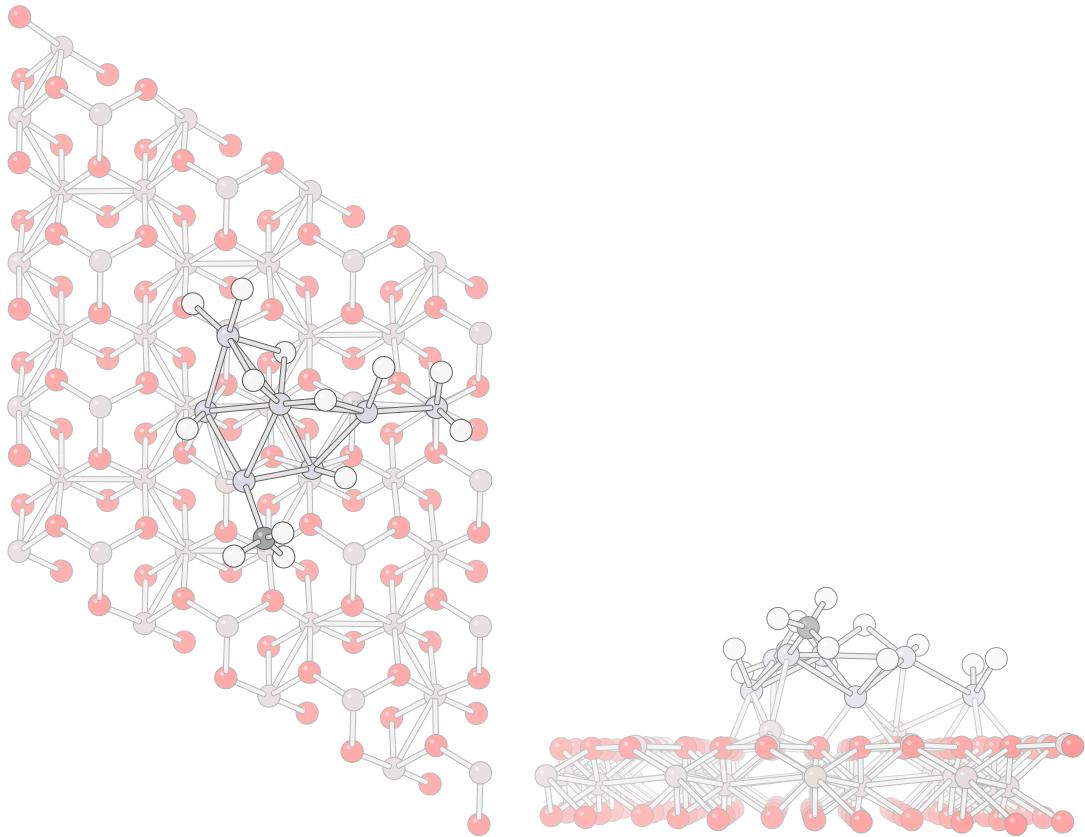
[Relax] Time: 23:39 Step: 91

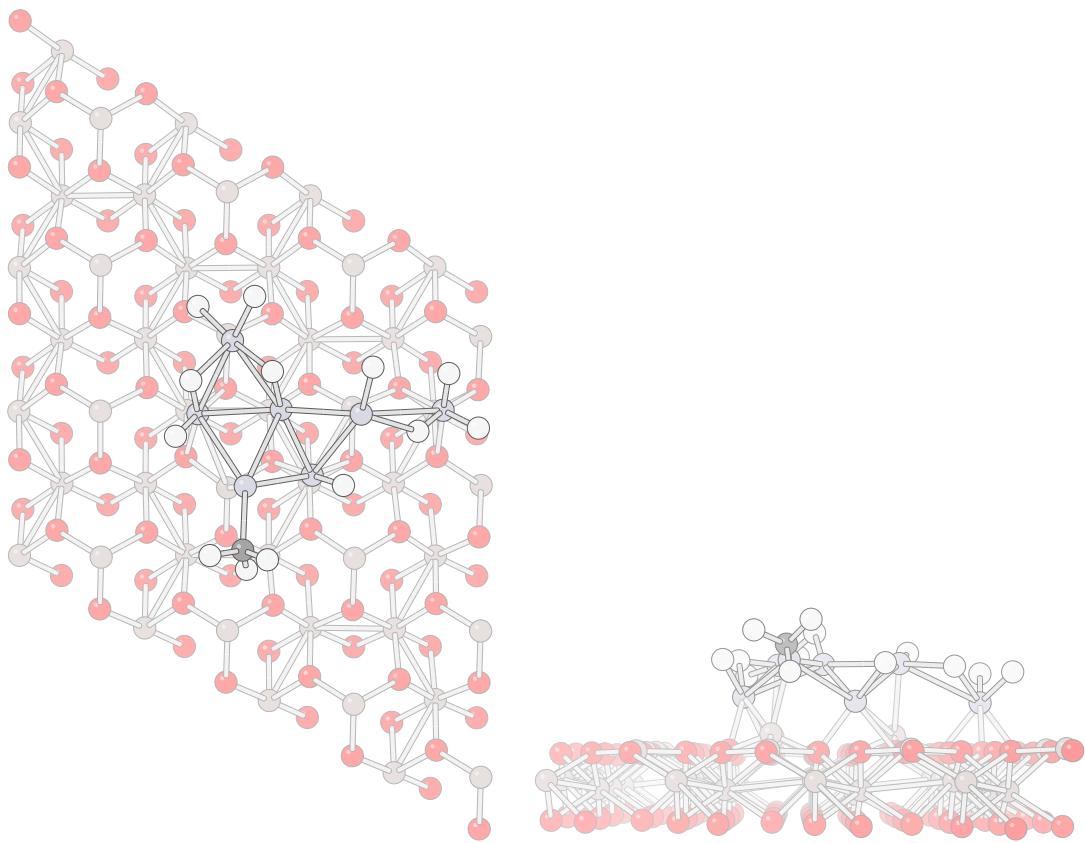


[8] ~ [1] (d = 0.40) #1.7.215 UNK (doublet)

E = -66.544680 (0.173 eV)

[Relax] Time: 32:28 Step: 144

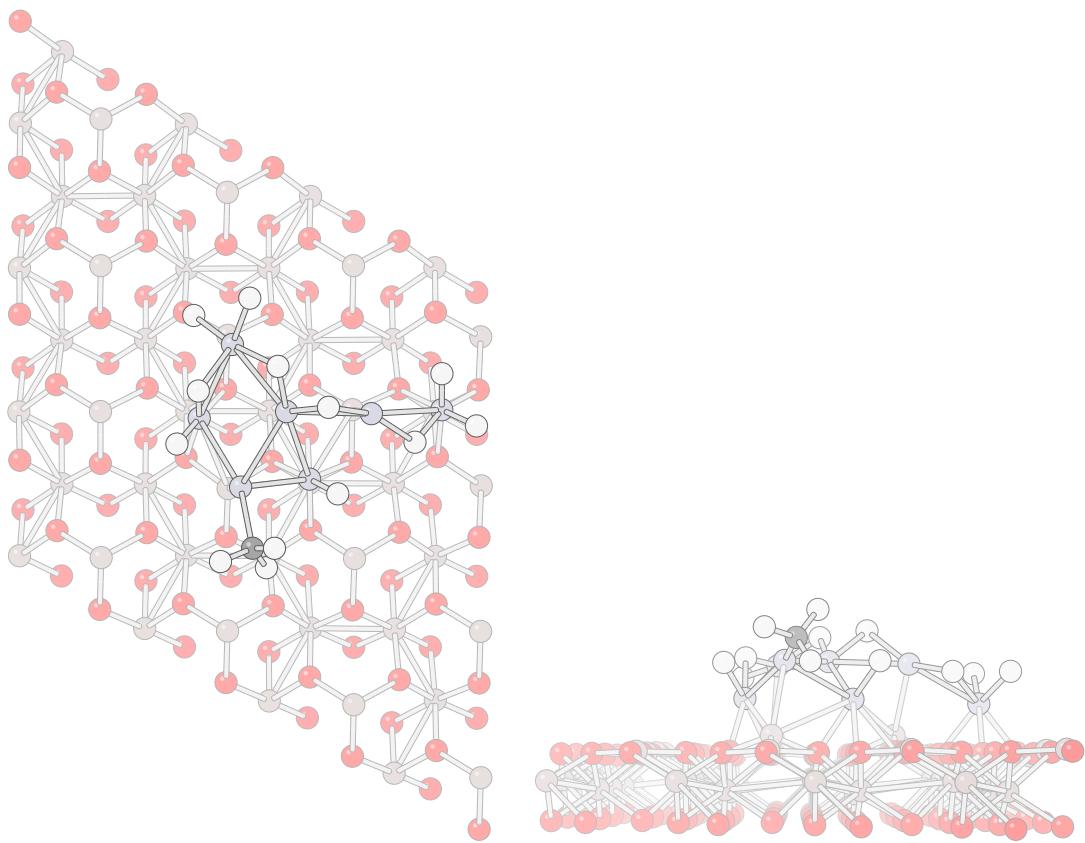




[11] ~ [1] (d = 0.34) #1.7.118 UNK (doublet)

E = -66.542555 (0.231 eV)

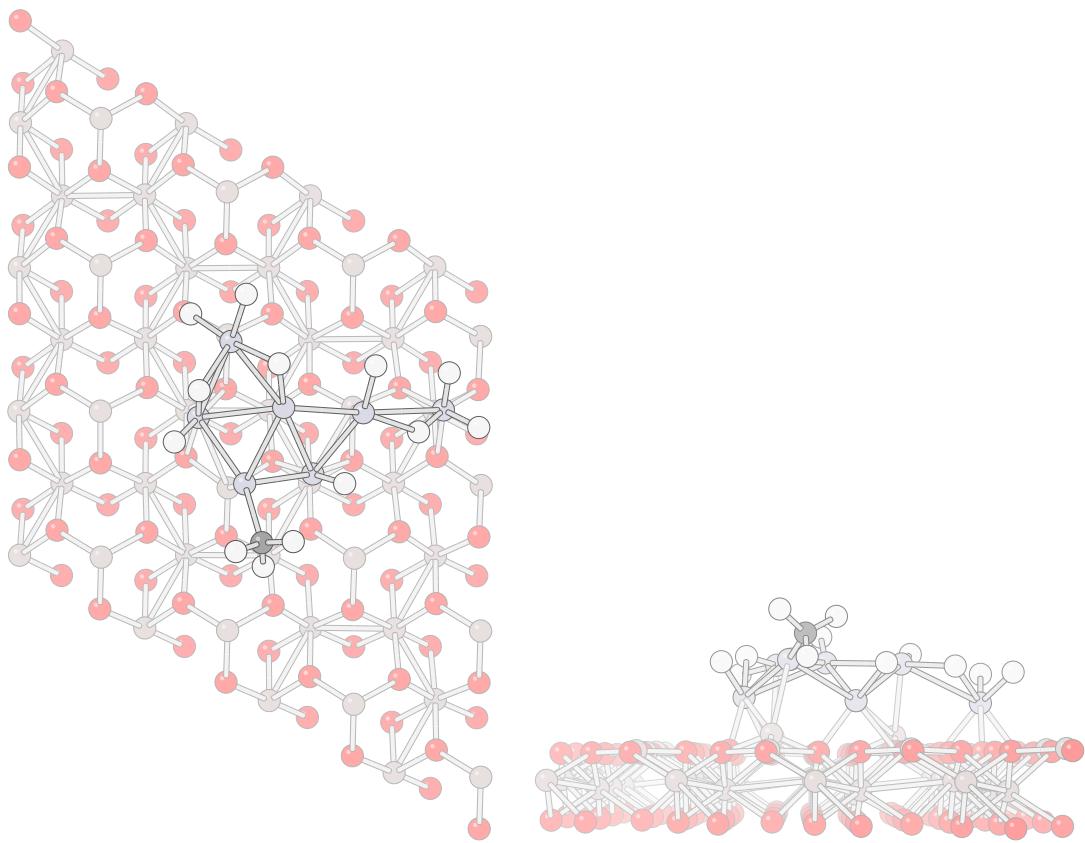
[Relax] Time: 26:33 Step: 127



[12] ~ [10] (d = 0.28) #1.7.288 UNK (doublet)

E = -66.542203 (0.241 eV)

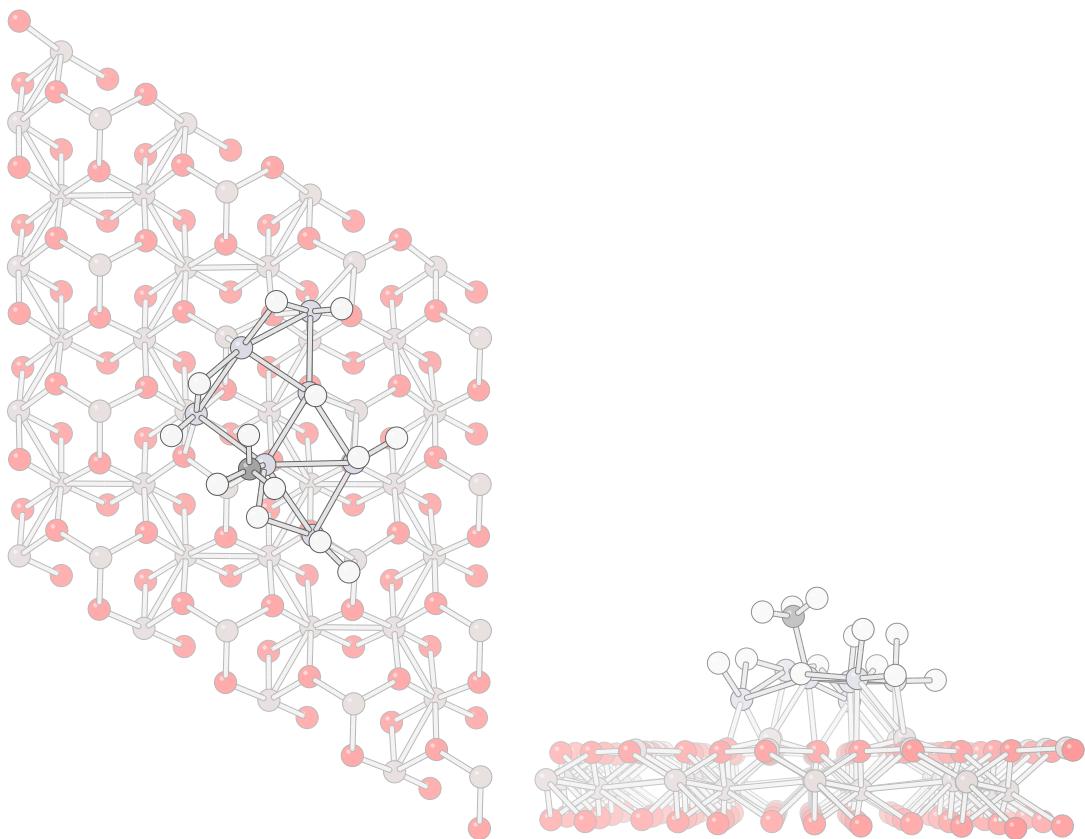
[Relax] Time: 25:44 Step: 111



[13] ~ [4] ($d = 1.49$) #1.0.172 UNK (doublet)

$E = -66.542032$ (0.245 eV)

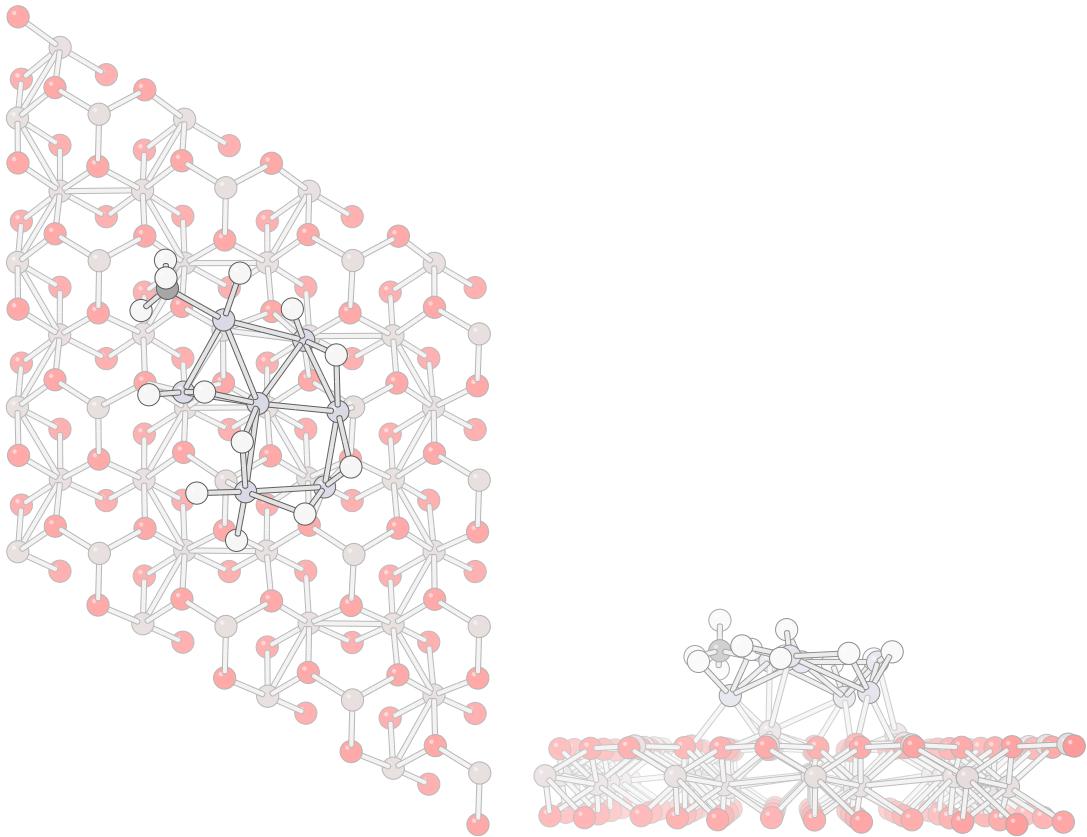
[Relax] Time: 30:55 Step: 147



[14] ~ [4] ($d = 0.31$) #1.3.124 UNK (doublet)

$E = -66.541563$ (0.258 eV)

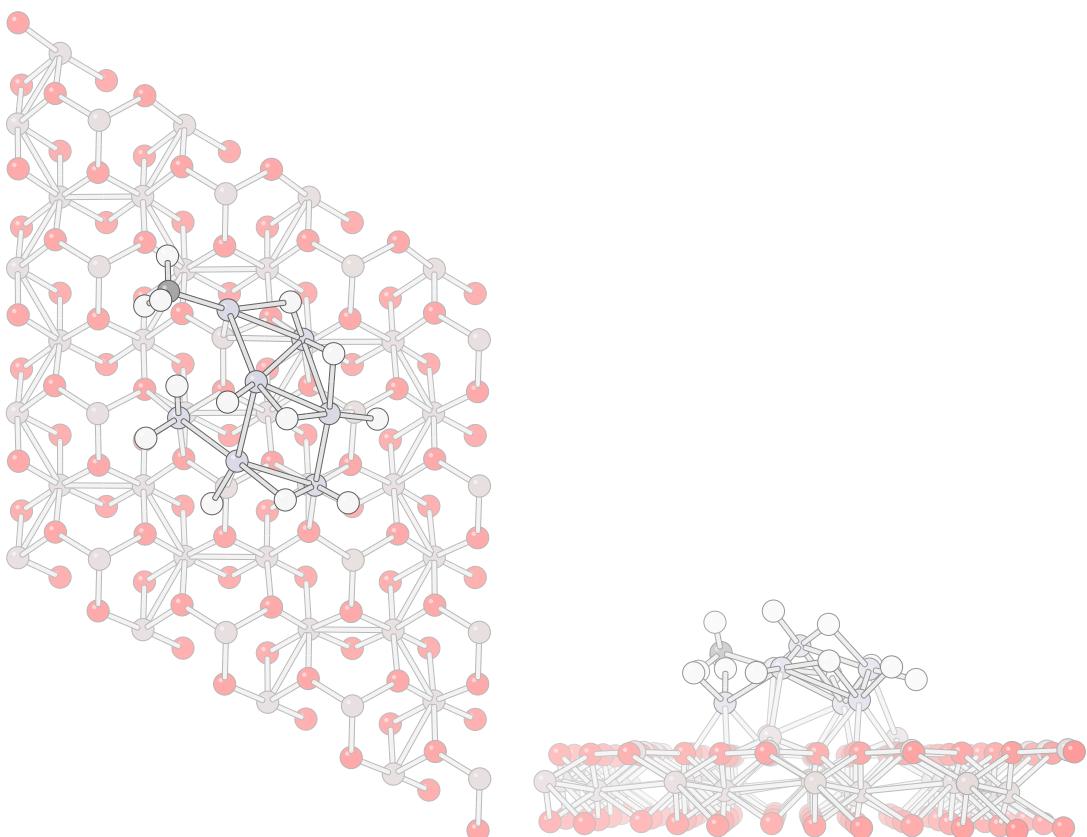
[Relax] Time: 43:51 Step: 176



[15] ~ [9] ($d = 0.91$) #1.3.209 UNK (mixed)

$E = -66.541182$ (0.268 eV)

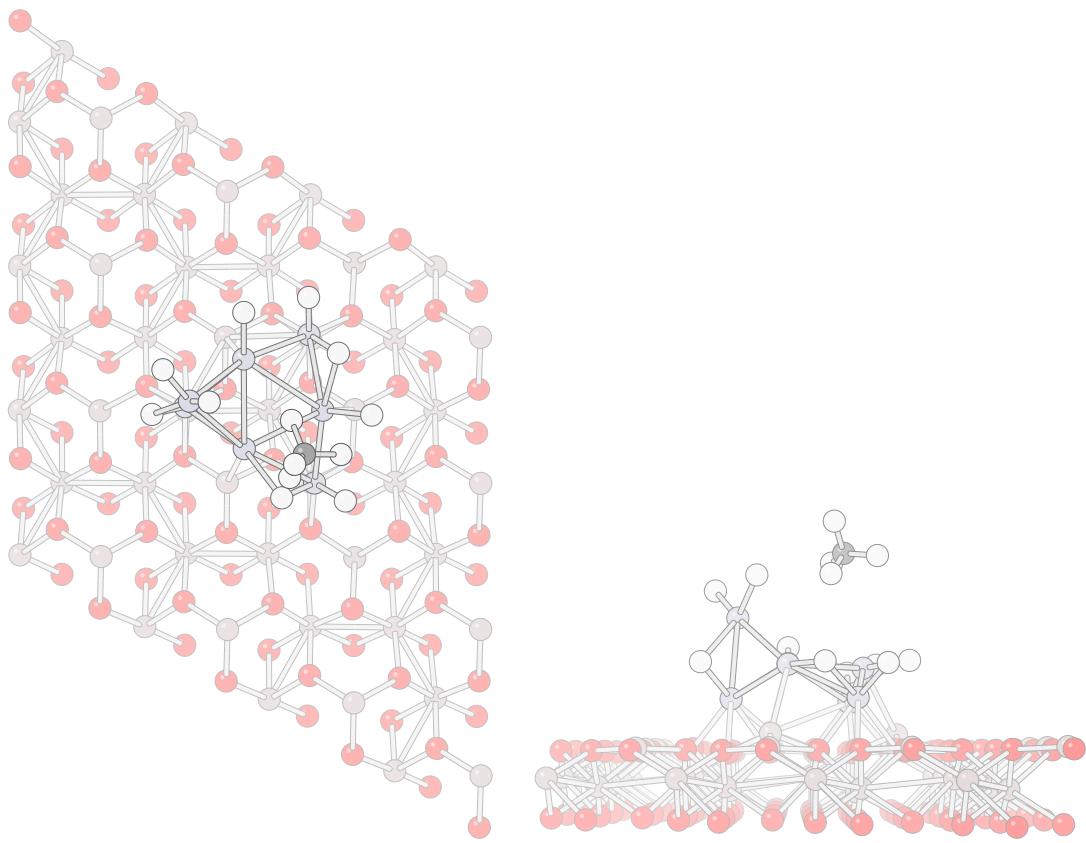
[Relax] Time: 20:16 Step: 85



[16] ~ [15] ($d = 1.71$) #1.5.65 UNK (mixed)

$E = -66.540603$ (0.284 eV)

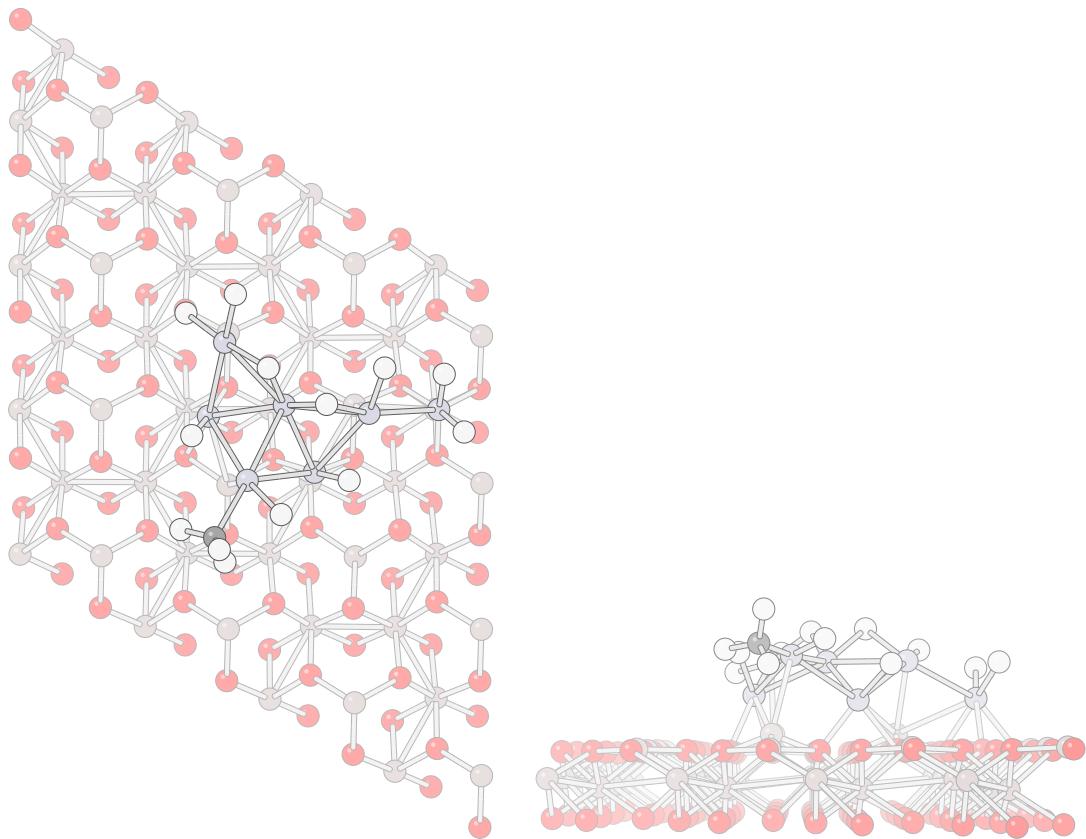
[Relax] Time: 47:20 Step: 135



[17] ~ [2] ($d = 0.52$) **#1.7.122** UNK (doublet)

E = -66.539927 (0.302 eV)

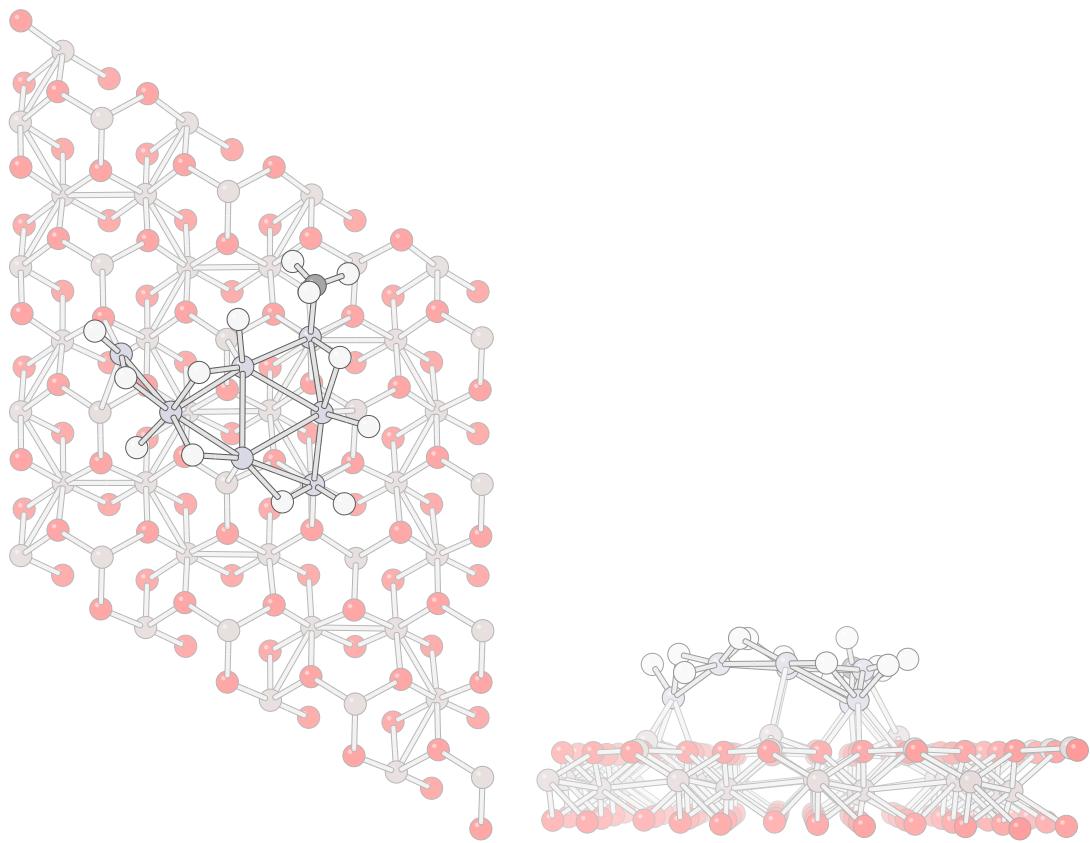
[Relax] Time: 40:42 Step: 200



[18] ~ [6] ($d = 0.79$) **#1.8.259** UNK (doublet)

E = -66.539893 (0.303 eV)

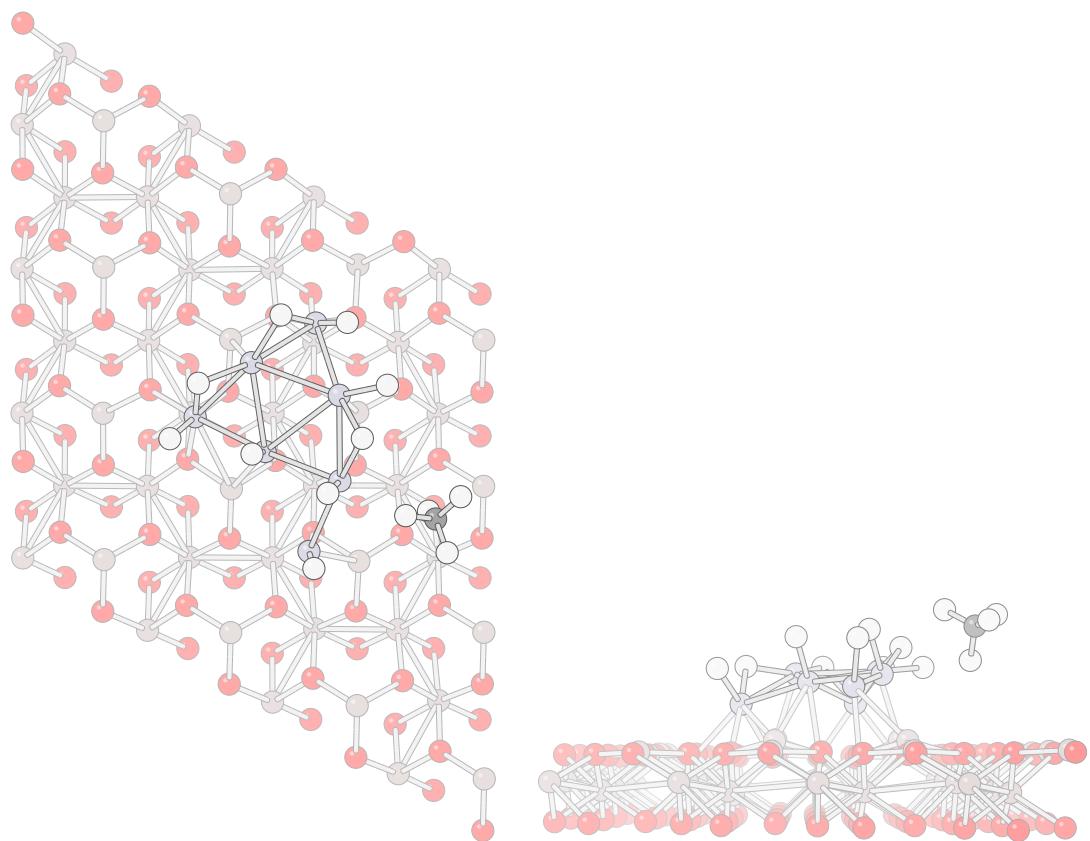
[Relax] Time: 21:44 Step: 97



[19] ~ [13] (d = 1.66) #1.0.287 UNK (doublet)

E = -66.539828 (0.305 eV)

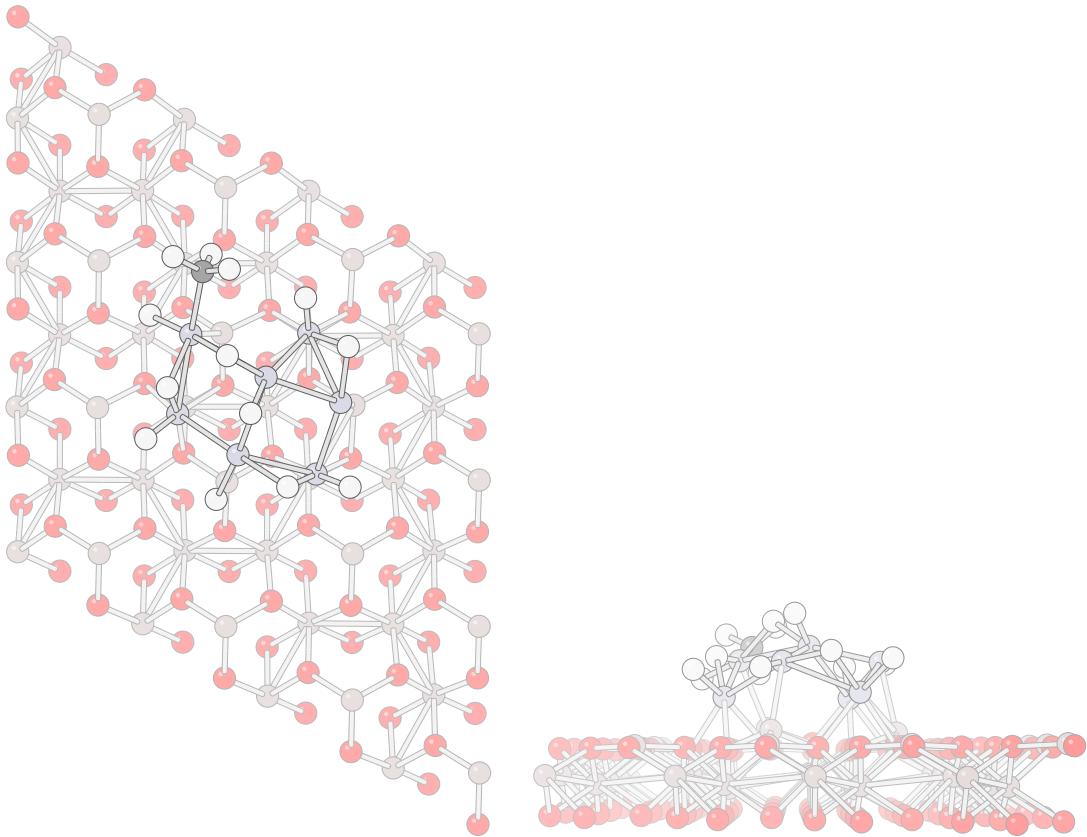
[Relax] Time: 30:57 Step: 148



[20] ~ [9] (d = 0.34) #1.3.285 UNK (doublet)

E = -66.539674 (0.309 eV)

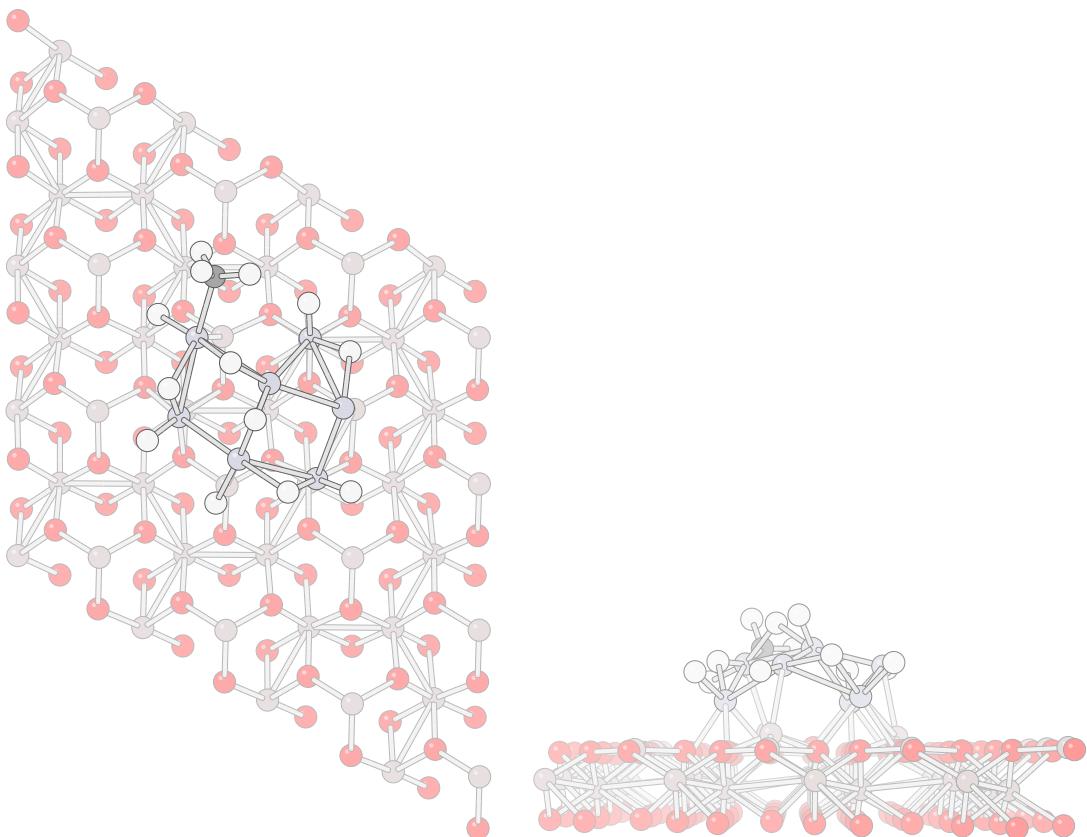
[Relax] Time: 23:14 Step: 90



[21] ~ [20] (d = 0.27) #1.3.278 UNK (doublet)

E = -66.539562 (0.312 eV)

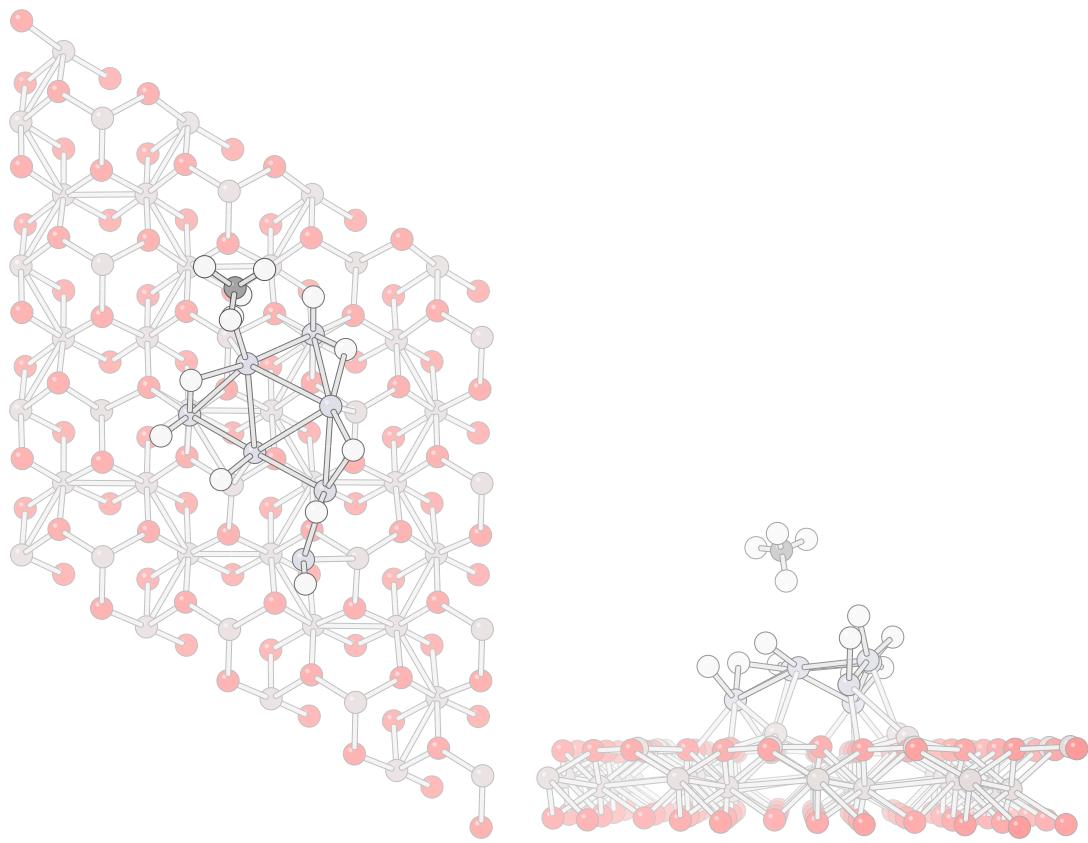
[Relax] Time: 19:25 Step: 81



[22] ~ [16] (d = 1.34) #1.8.201 UNK (doublet)

E = -66.539416 (0.316 eV)

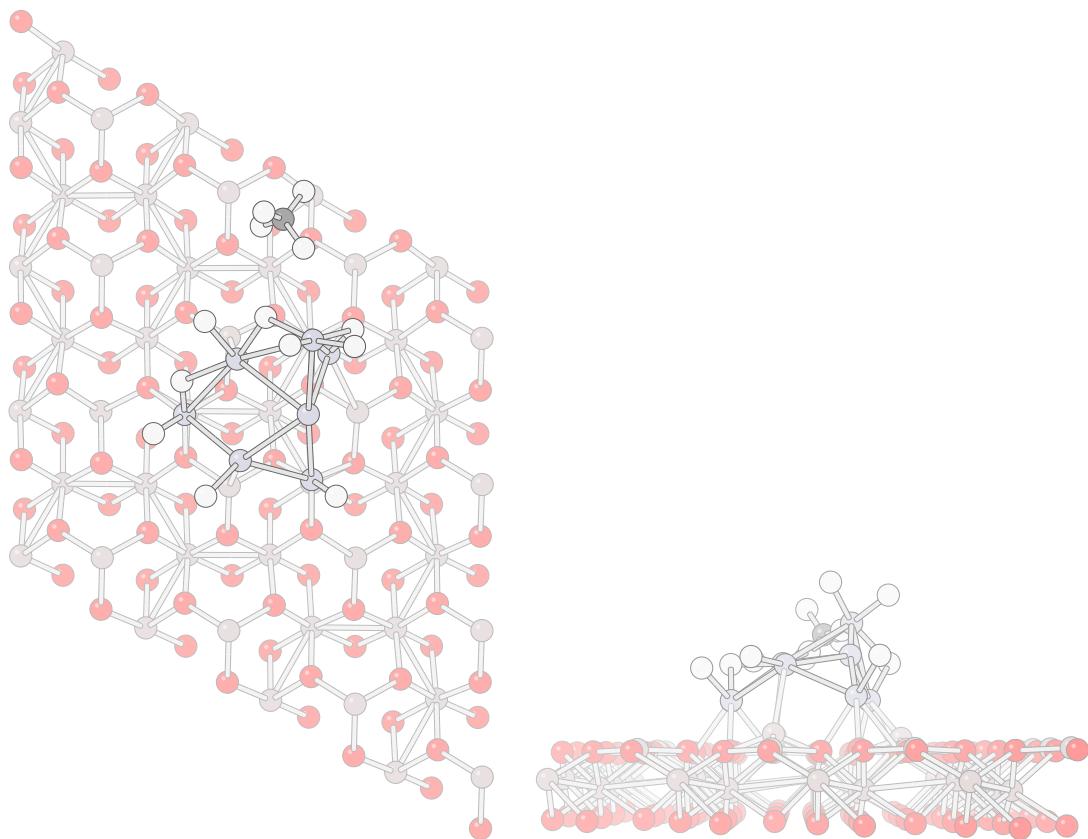
[Relax] Time: 53:16 Step: 236



[23] ~ [19] ($d = 0.98$) #1.8.125 UNK (doublet)

E = -66.539377 (0.317 eV)

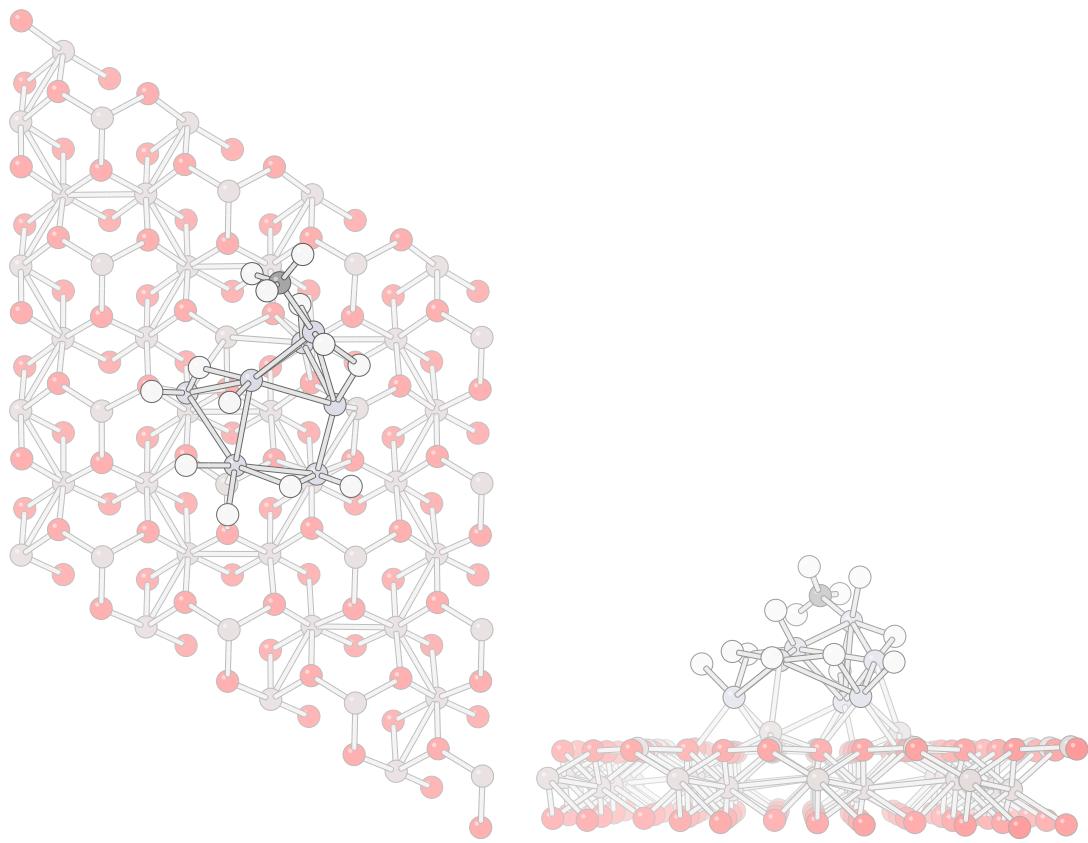
[Relax] Time: 1:03:58 Step: 250



[24] ~ [9] ($d = 1.25$) #1.5.258 UNK (doublet)

E = -66.539074 (0.326 eV)

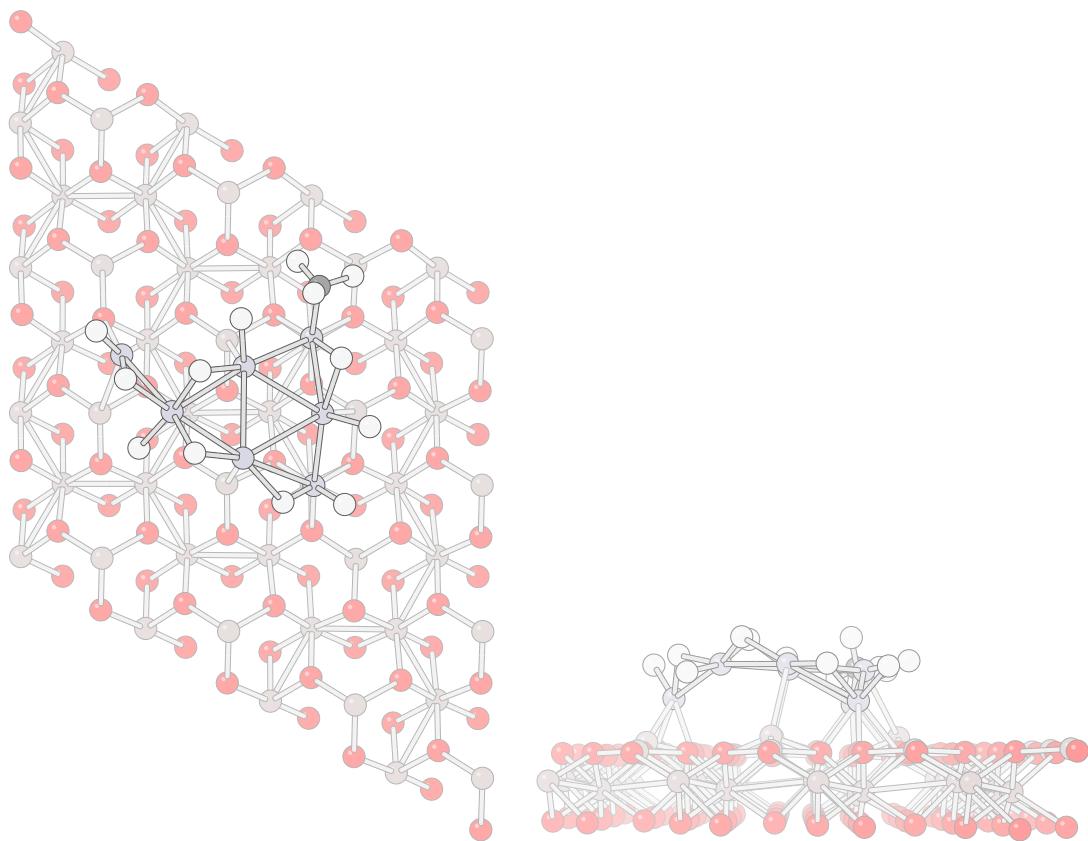
[Relax] Time: 20:47 Step: 87



[25] ~ [18] ($d = 0.54$) #1.8.262 UNK (doublet)

$E = -66.538944$ (0.329 eV)

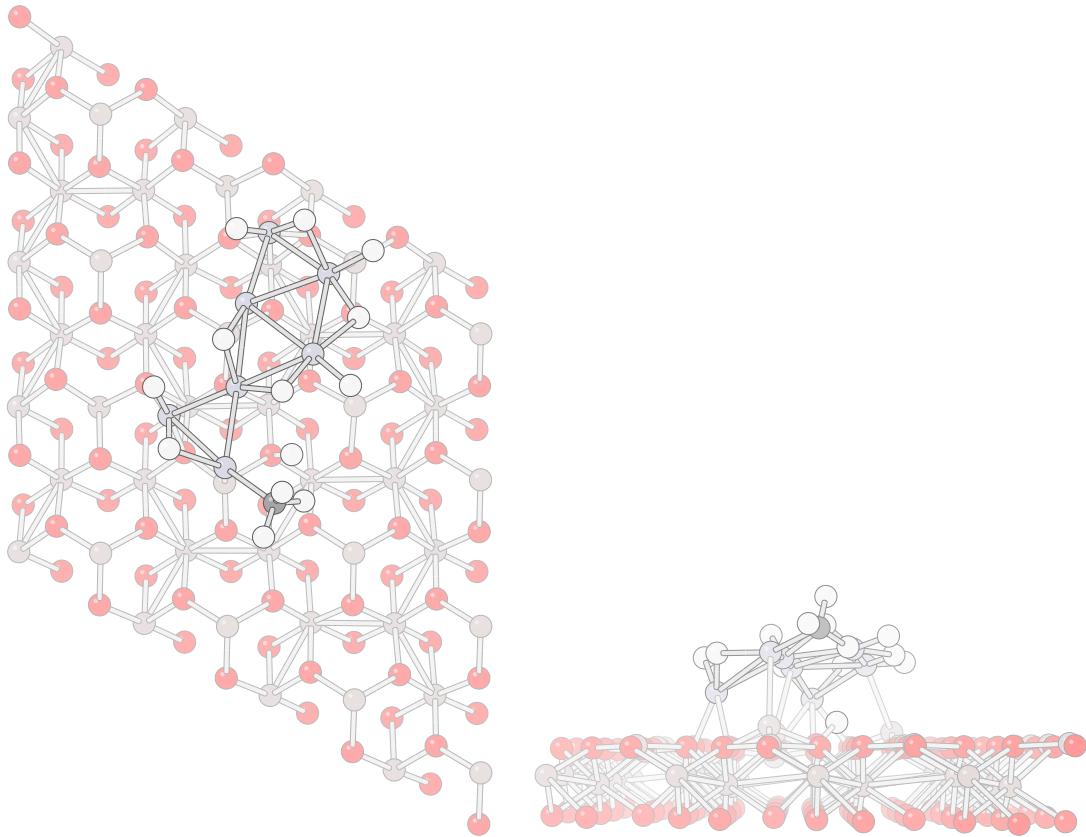
[Relax] Time: 42:29 Step: 202



[26] ~ [13] ($d = 1.79$) #1.6.81 UNK (doublet)

$E = -66.538876$ (0.331 eV)

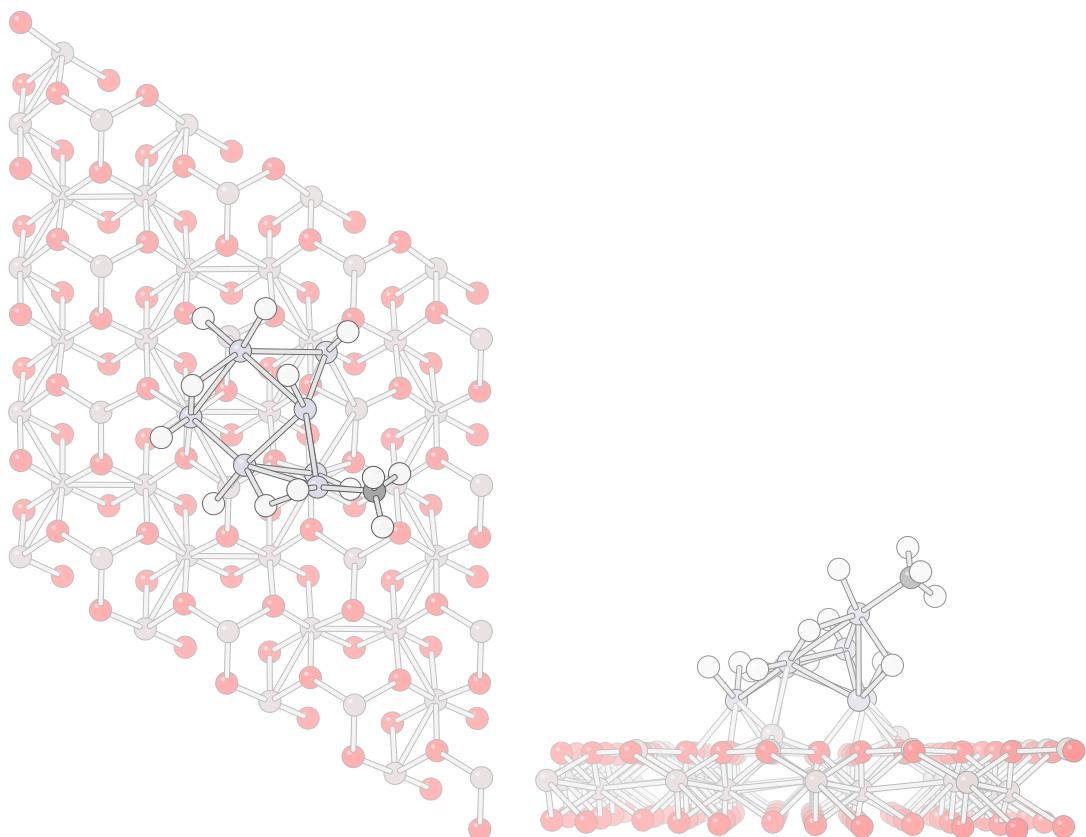
[Relax] Time: 58:19 Step: 202



[27] ~ [24] (d = 0.48) #1.5.205 UNK (doublet)

E = -66.537989 (0.355 eV)

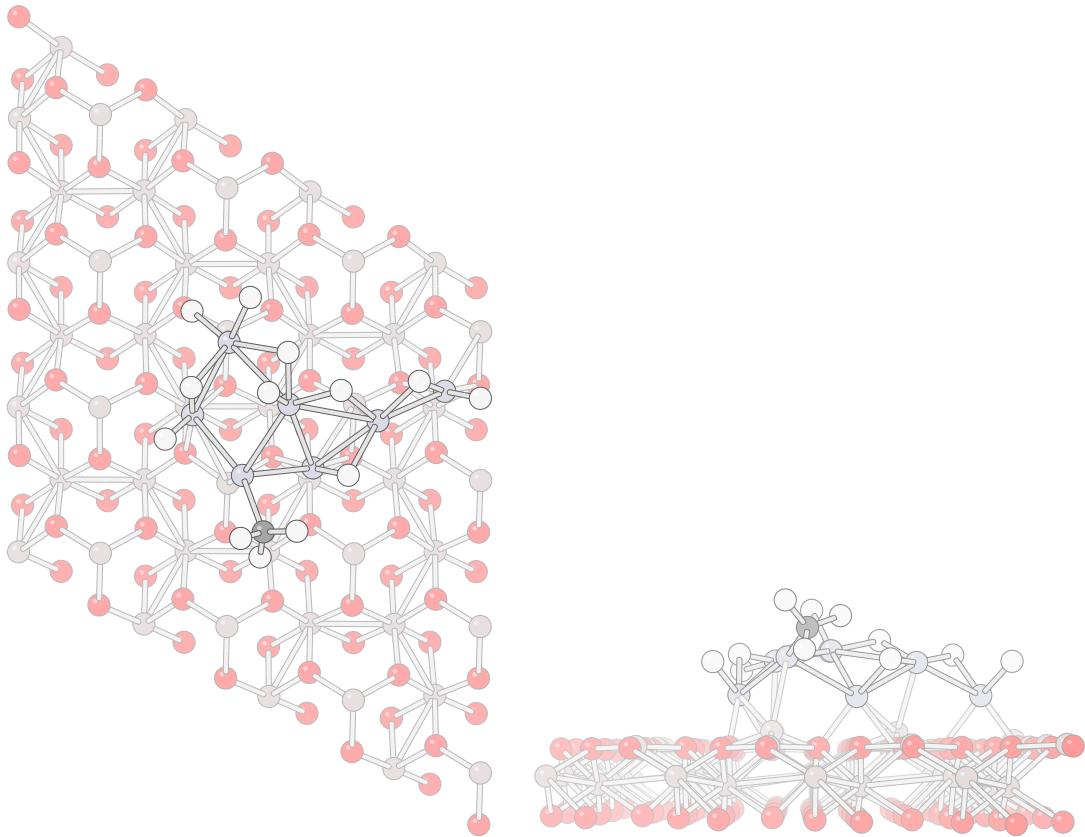
[Relax] Time: 25:05 Step: 116



[28] ~ [3] (d = 0.41) #1.7.231 UNK (doublet)

E = -66.537914 (0.357 eV)

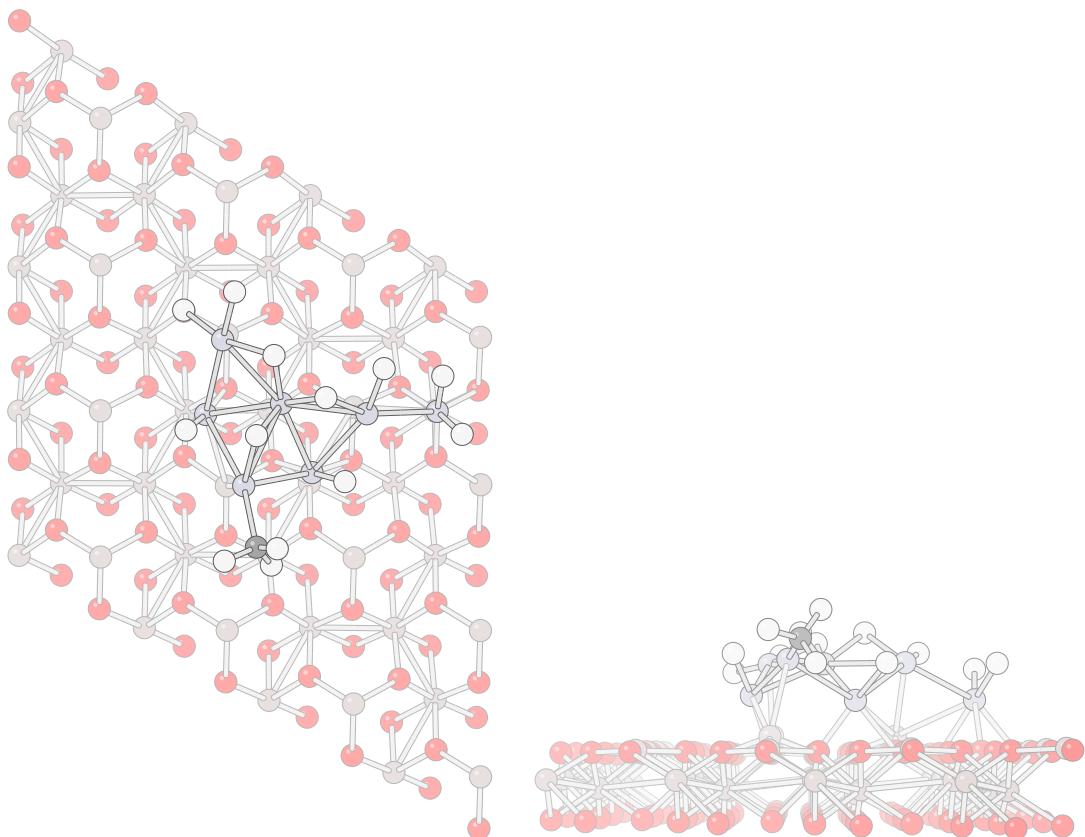
[Relax] Time: 20:09 Step: 94



[29] ~ [8] ($d = 0.29$) #1.7.146 UNK (doublet)

$E = -66.537747$ (0.362 eV)

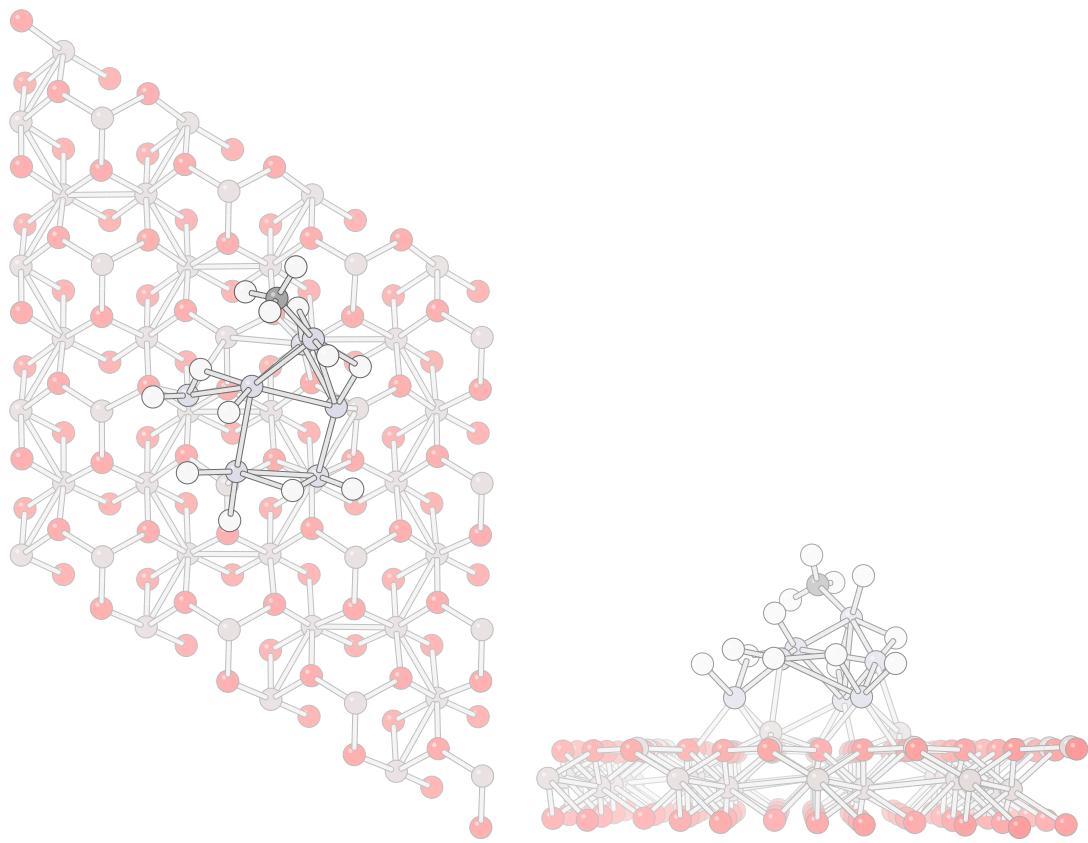
[Relax] Time: 33:05 Step: 149



[30] ~ [24] ($d = 0.27$) #1.5.255 UNK (doublet)

$E = -66.537729$ (0.362 eV)

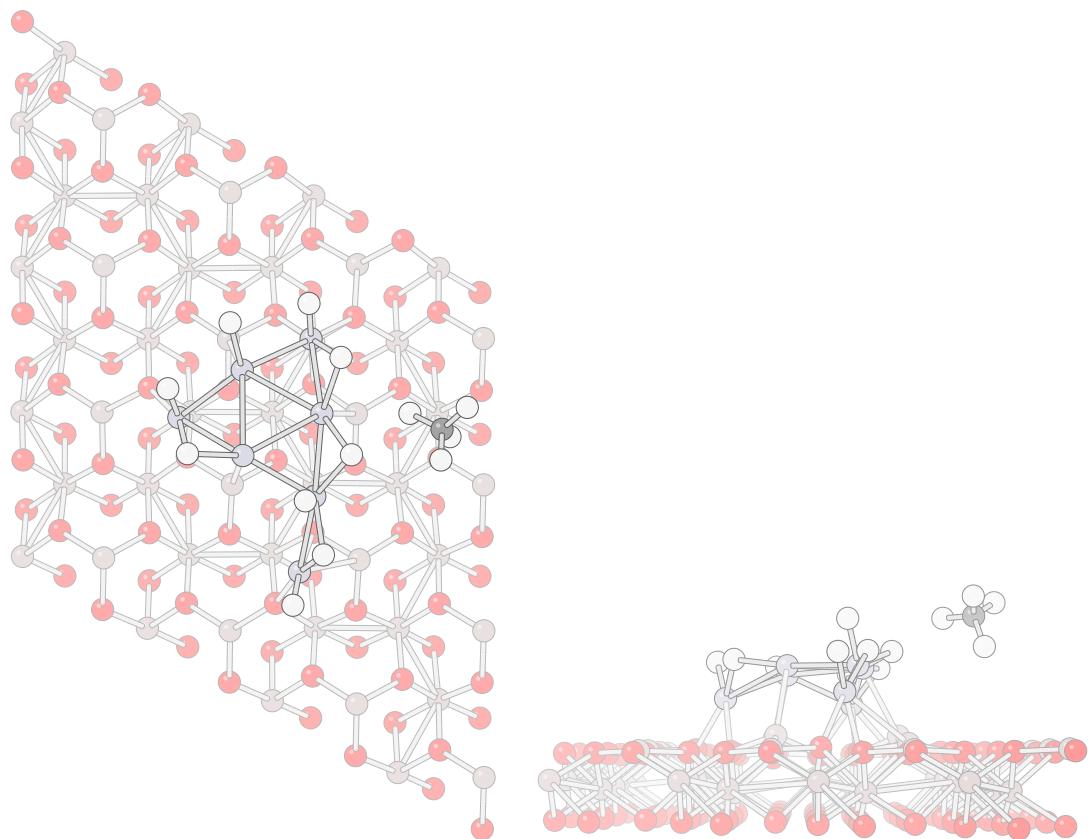
[Relax] Time: 17:18 Step: 73



[31] ~ [21] (d = 1.42) #1.8.284 UNK (doublet)

E = -66.537134 (0.378 eV)

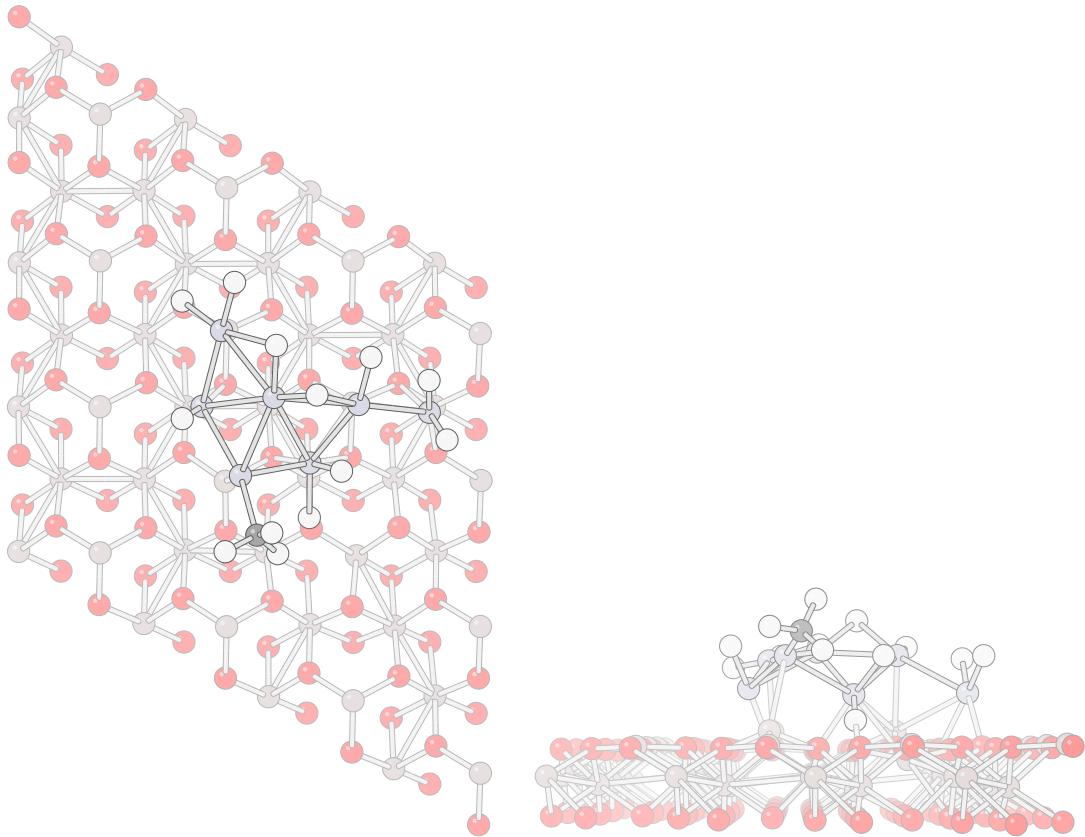
[Relax] Time: 54:29 Step: 234



[32] ~ [29] (d = 0.51) #1.7.101 UNK (doublet)

E = -66.535792 (0.415 eV)

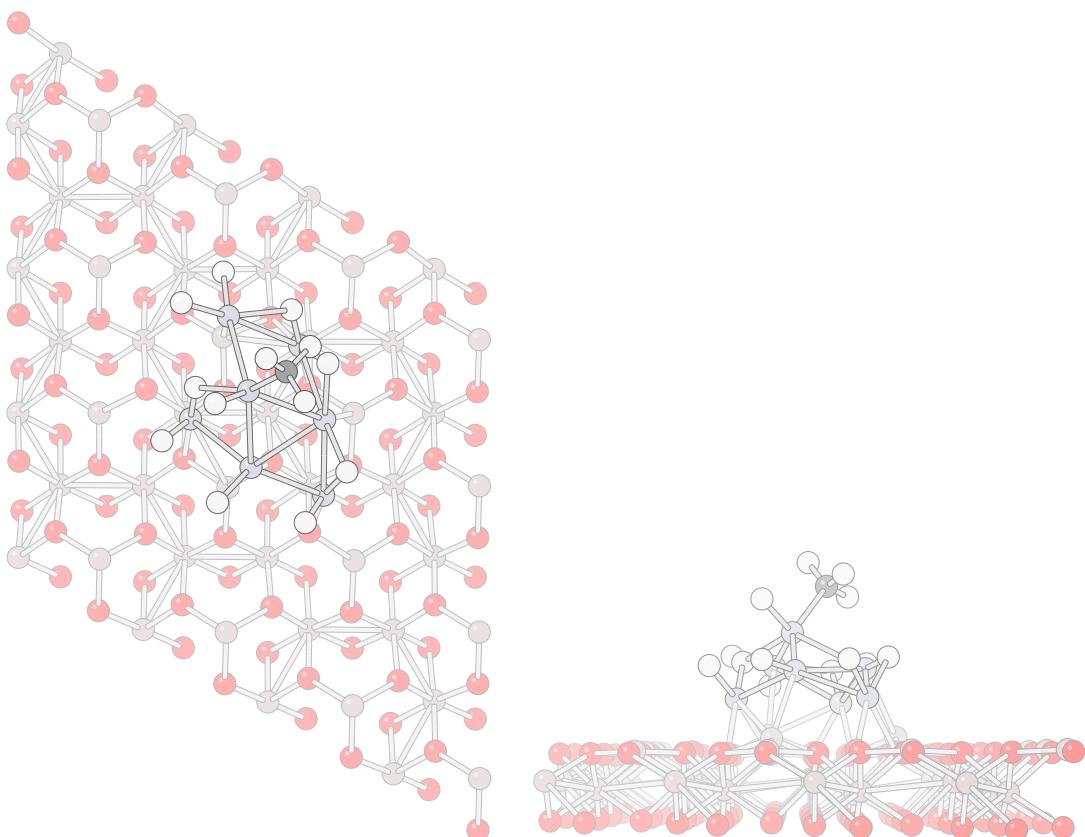
[Relax] Time: 59:18 Step: 202



[33] ~ [15] (d = 1.23) #1.9.250 UNK (doublet)

E = -66.535377 (0.426 eV)

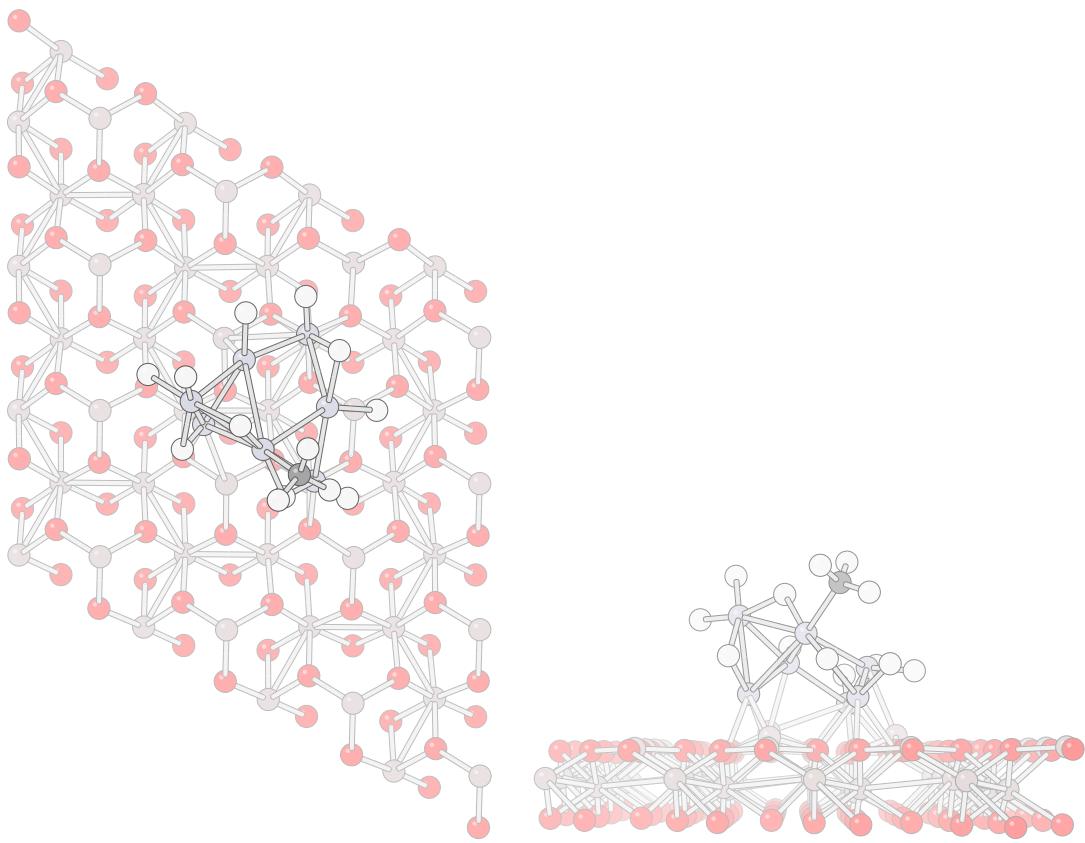
[Relax] Time: 17:32 Step: 80



[34] ~ [16] (d = 0.67) #1.5.153 UNK (doublet)

E = -66.535208 (0.431 eV)

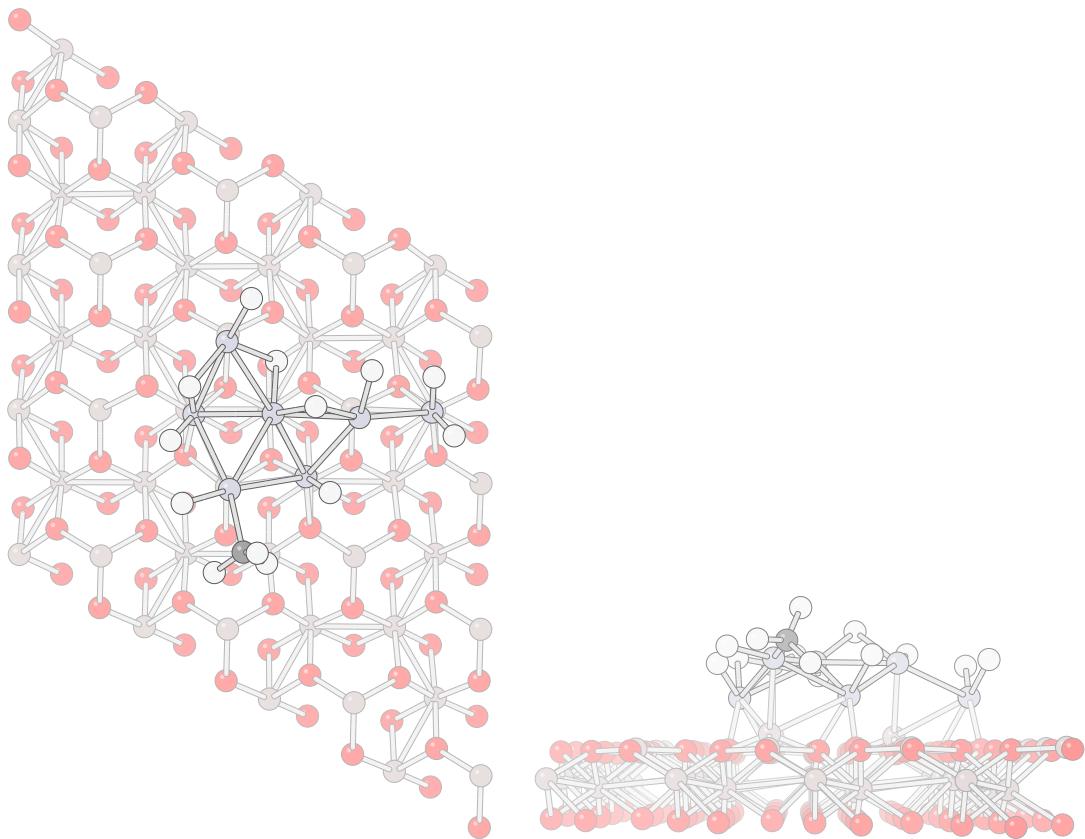
[Relax] Time: 24:31 Step: 100



[35] ~ [1] ($d = 0.62$) #1.7.155 UNK (doublet)

$E = -66.535018$ (0.436 eV)

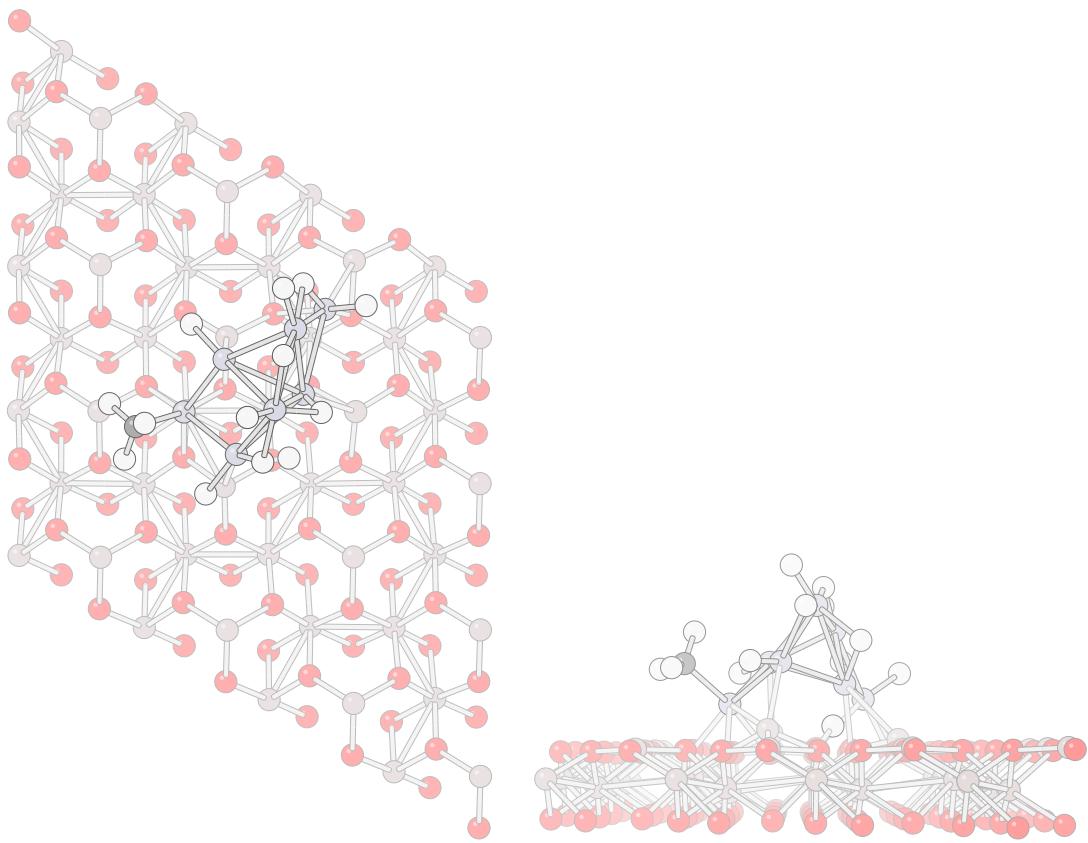
[Relax] Time: 20:16 Step: 89



[36] ~ [34] ($d = 1.75$) #1.2.197 UNK (doublet)

$E = -66.534592$ (0.448 eV)

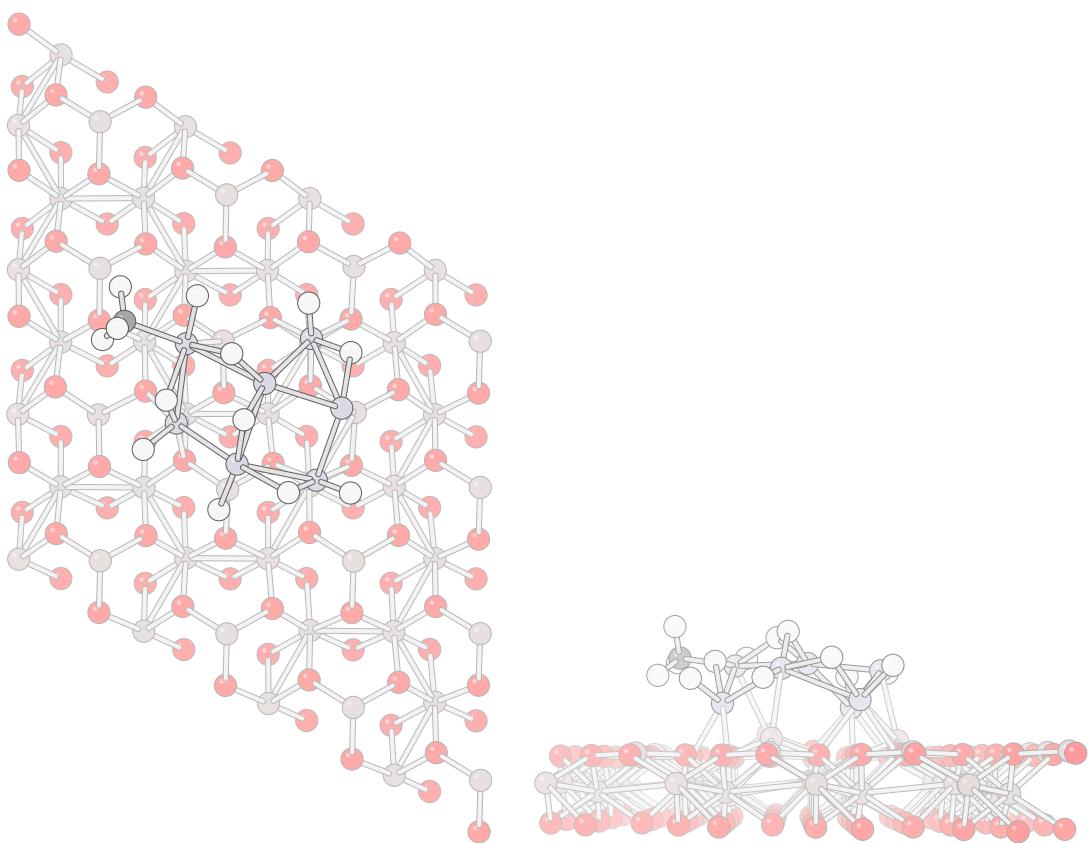
[Relax] Time: 24:20 Step: 105



[37] ~ [20] (d = 0.68) #1.3.290 UNK (doublet)

E = -66.534309 (0.455 eV)

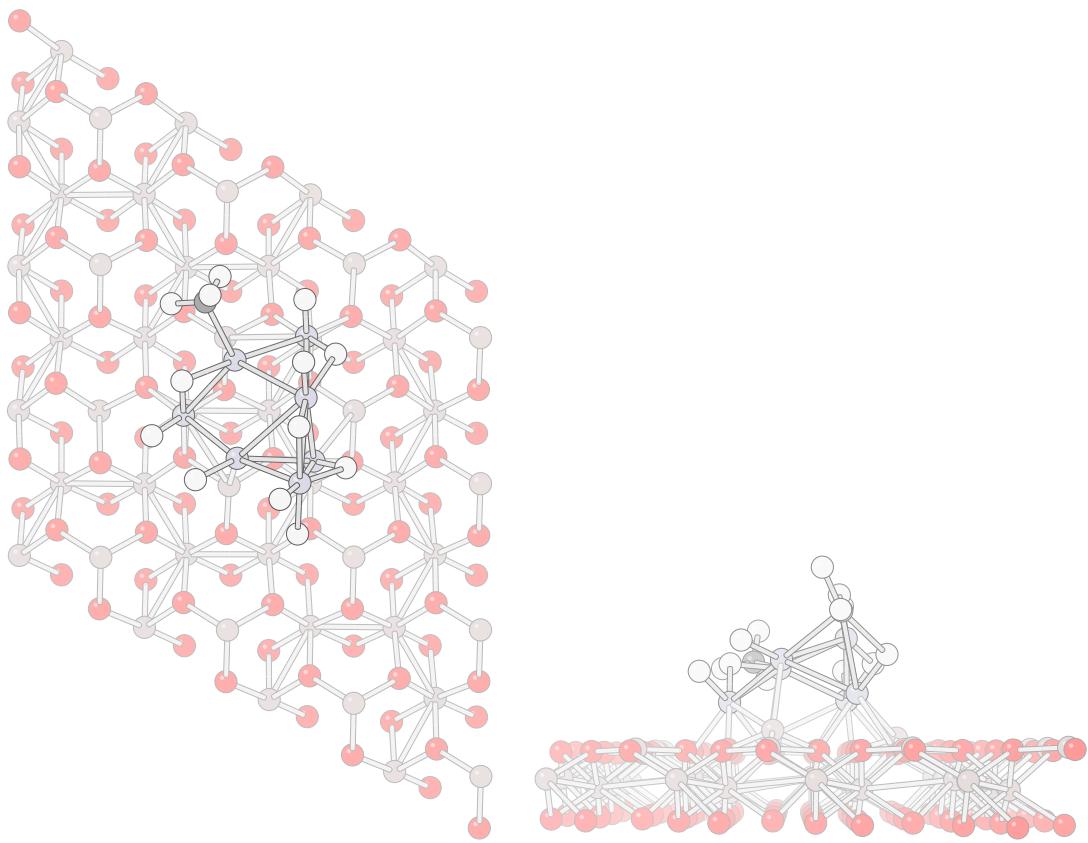
[Relax] Time: 1:06:10 Step: 271



[38] ~ [34] (d = 0.79) #1.9.152 UNK (doublet)

E = -66.534121 (0.460 eV)

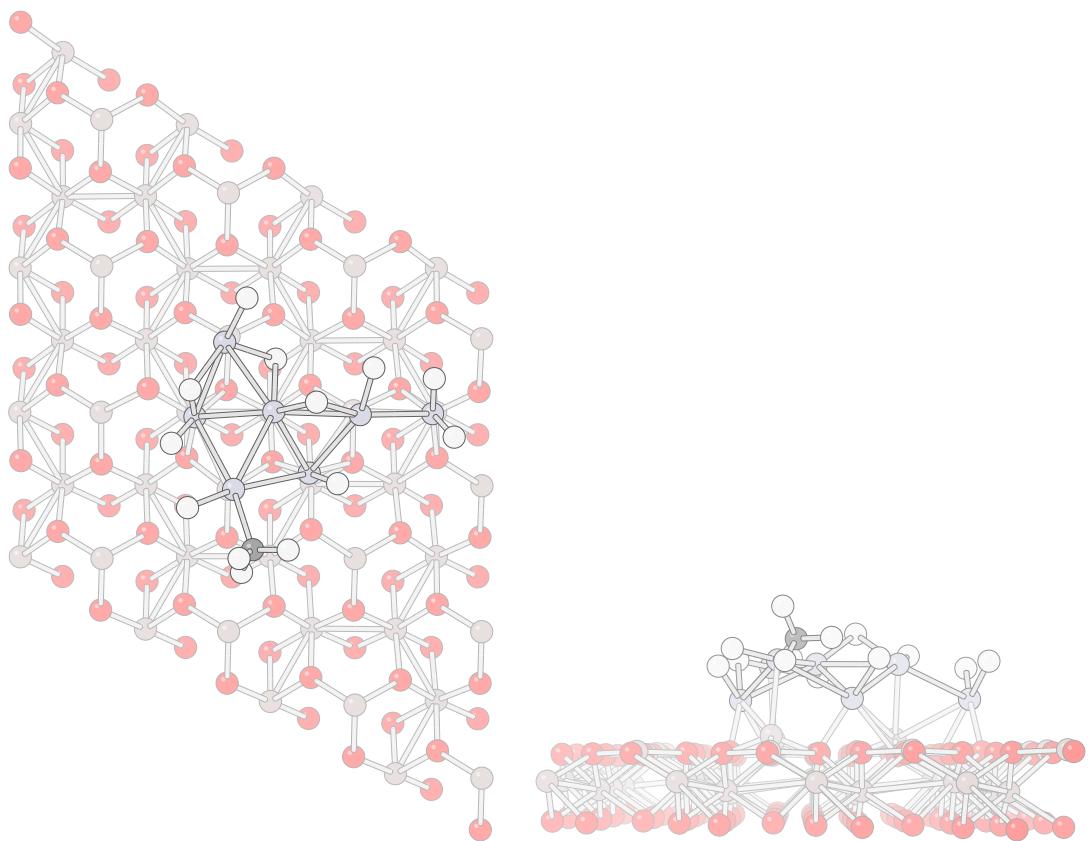
[Relax] Time: 25:07 Step: 97



[39] ~ [35] (d = 0.26) #1.7.205 UNK (doublet)

E = -66.533868 (0.467 eV)

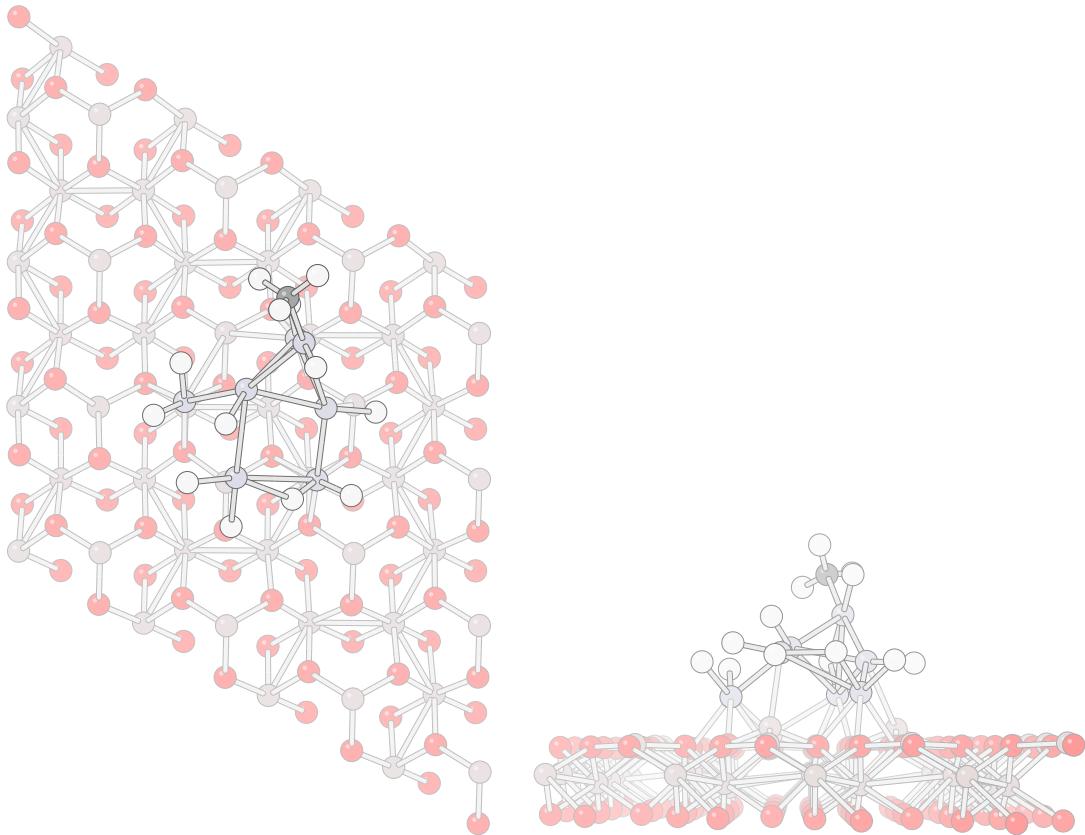
[Relax] Time: 24:51 Step: 116



[40] ~ [30] (d = 0.51) #1.5.254 UNK (doublet)

E = -66.533398 (0.480 eV)

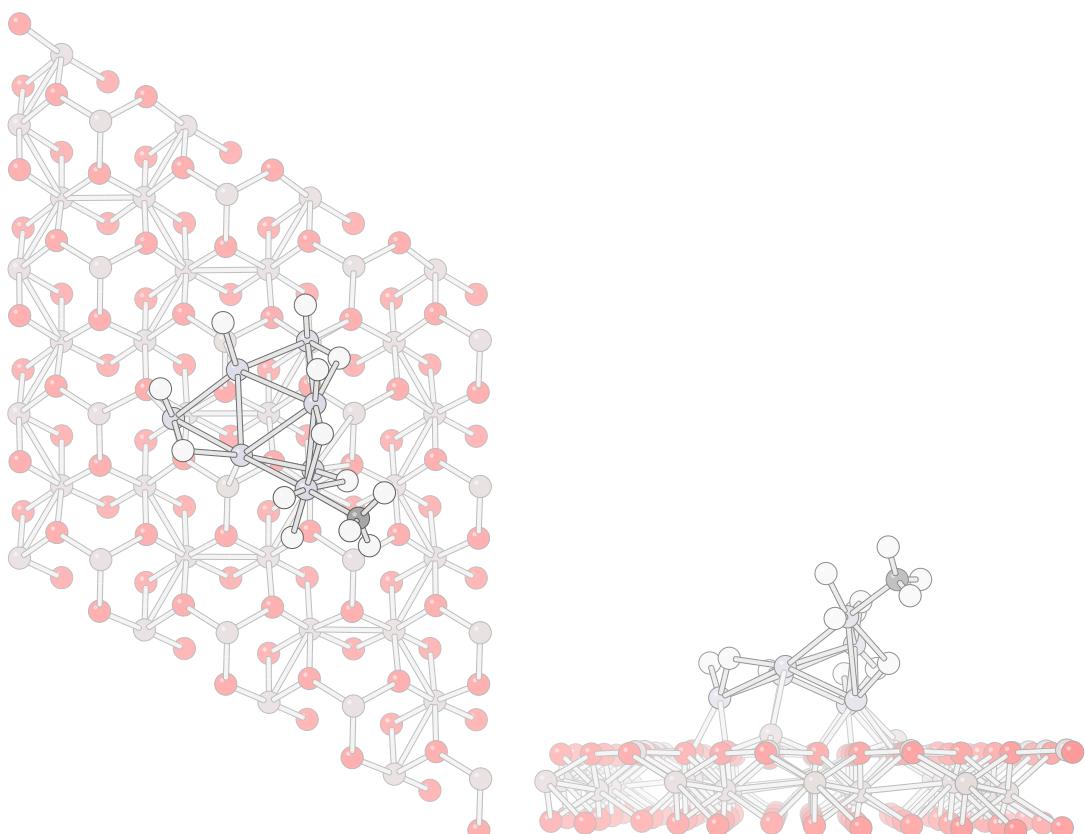
[Relax] Time: 32:47 Step: 152



[41] ~ [24] (d = 0.94) #1.9.140 UNK (doublet)

E = -66.533342 (0.482 eV)

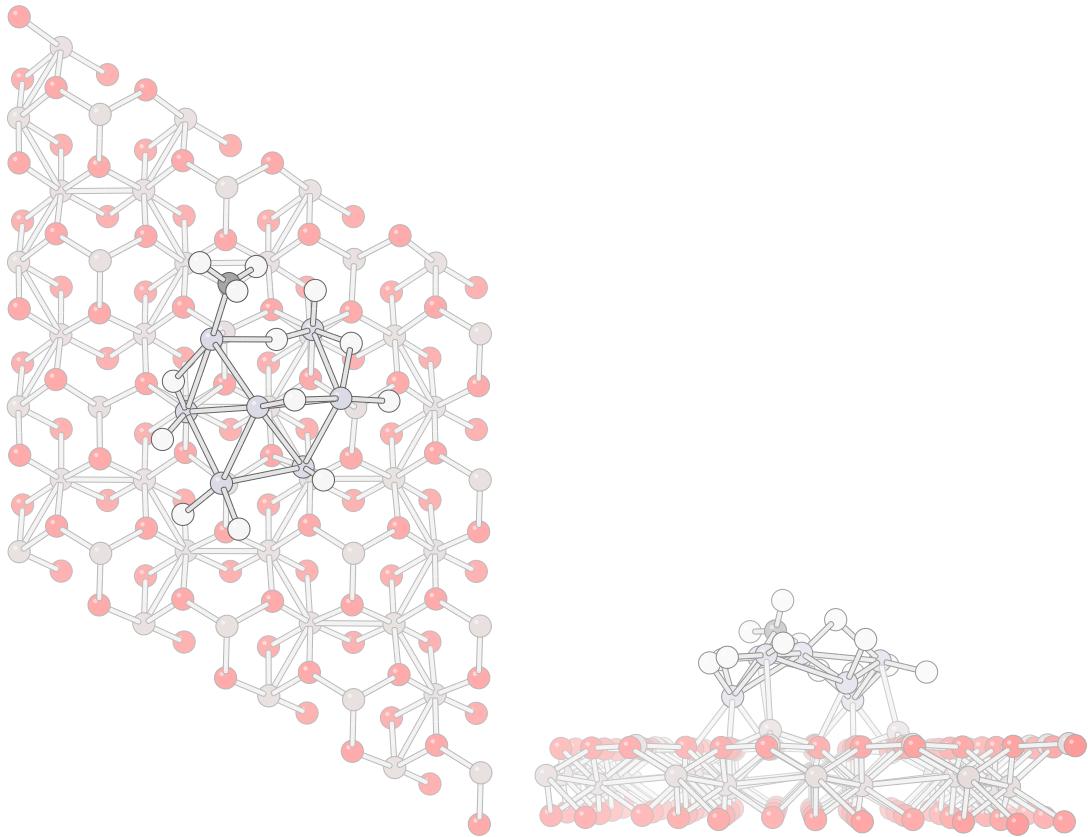
[Relax] Time: 31:37 Step: 126



[42] ~ [21] (d = 1.16) #1.3.159 UNK (doublet)

E = -66.533278 (0.483 eV)

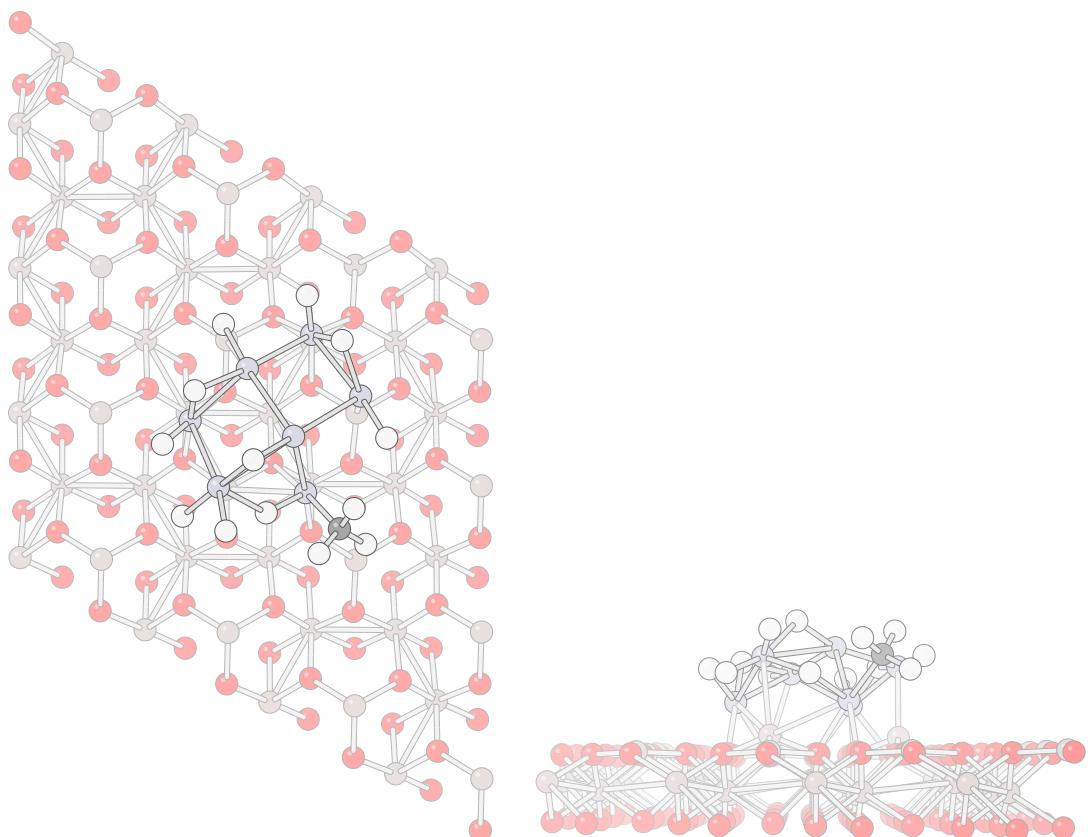
[Relax] Time: 1:07:25 Step: 270



[43] ~ [15] (d = 1.13) #1.3.71 UNK (doublet)

E = -66.533145 (0.487 eV)

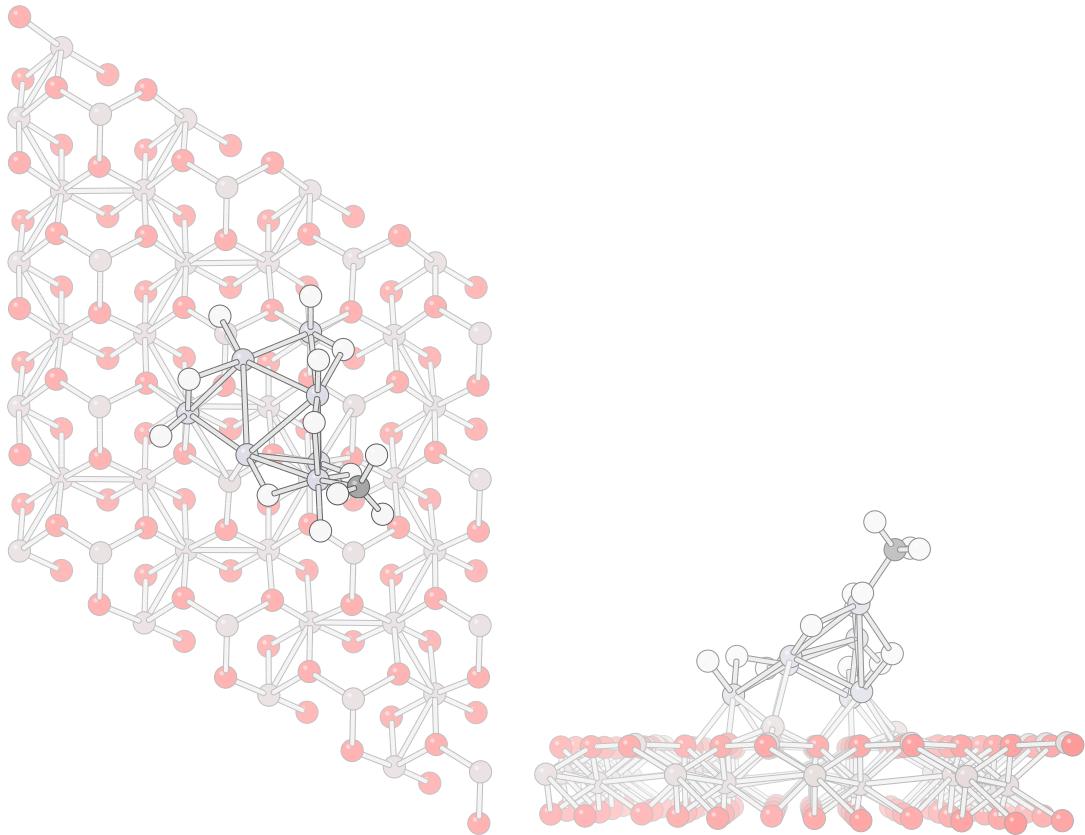
[Relax] Time: 28:20 Step: 116



[44] ~ [41] (d = 0.61) #1.9.147 UNK (doublet)

E = -66.532418 (0.507 eV)

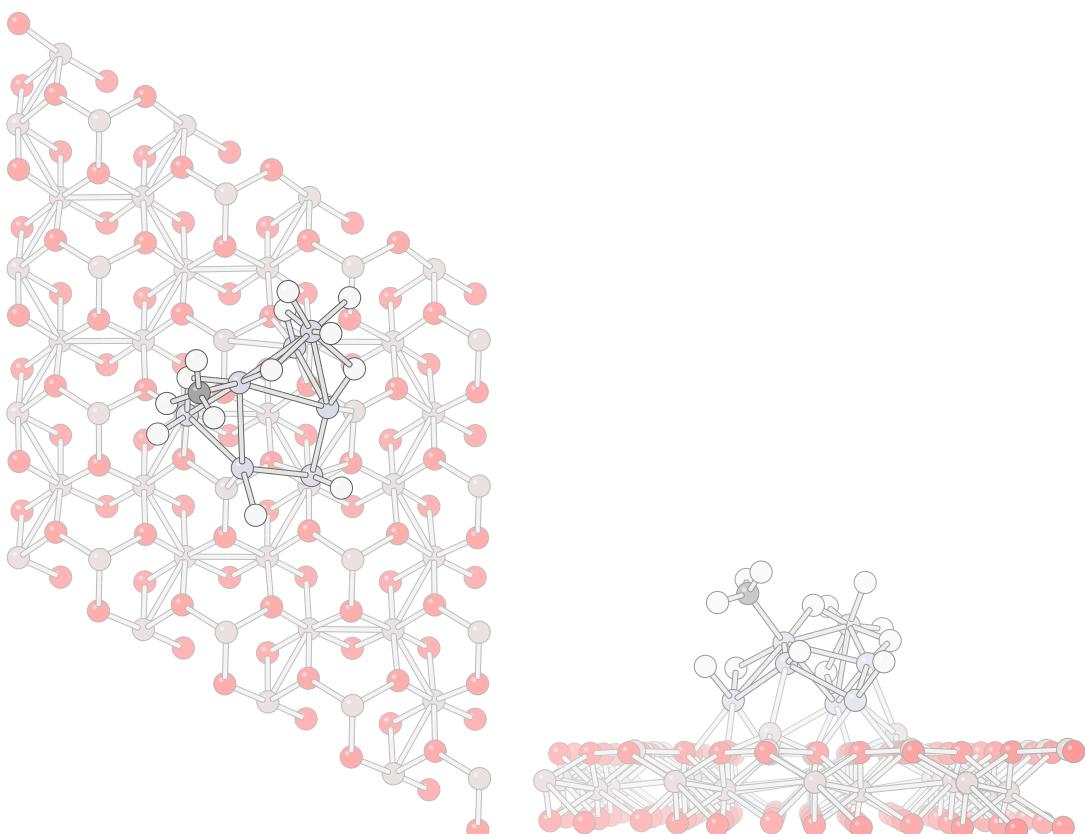
[Relax] Time: 45:36 Step: 191



[45] ~ [34] ($d = 0.84$) #1.5.26 UNK (doublet)

$E = -66.532254$ (0.511 eV)

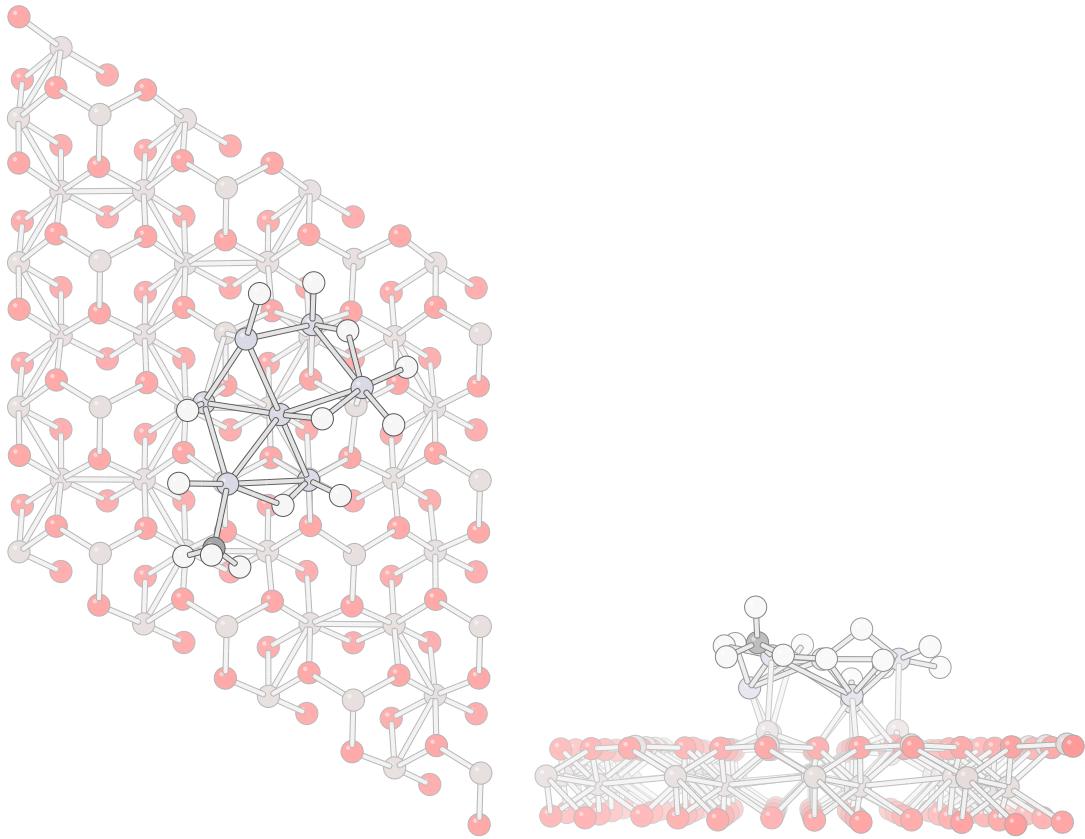
[Relax] Time: 1:28:38 Step: 347



[46] ~ [4] ($d = 0.46$) #1.3.116 UNK (doublet)

$E = -66.532174$ (0.513 eV)

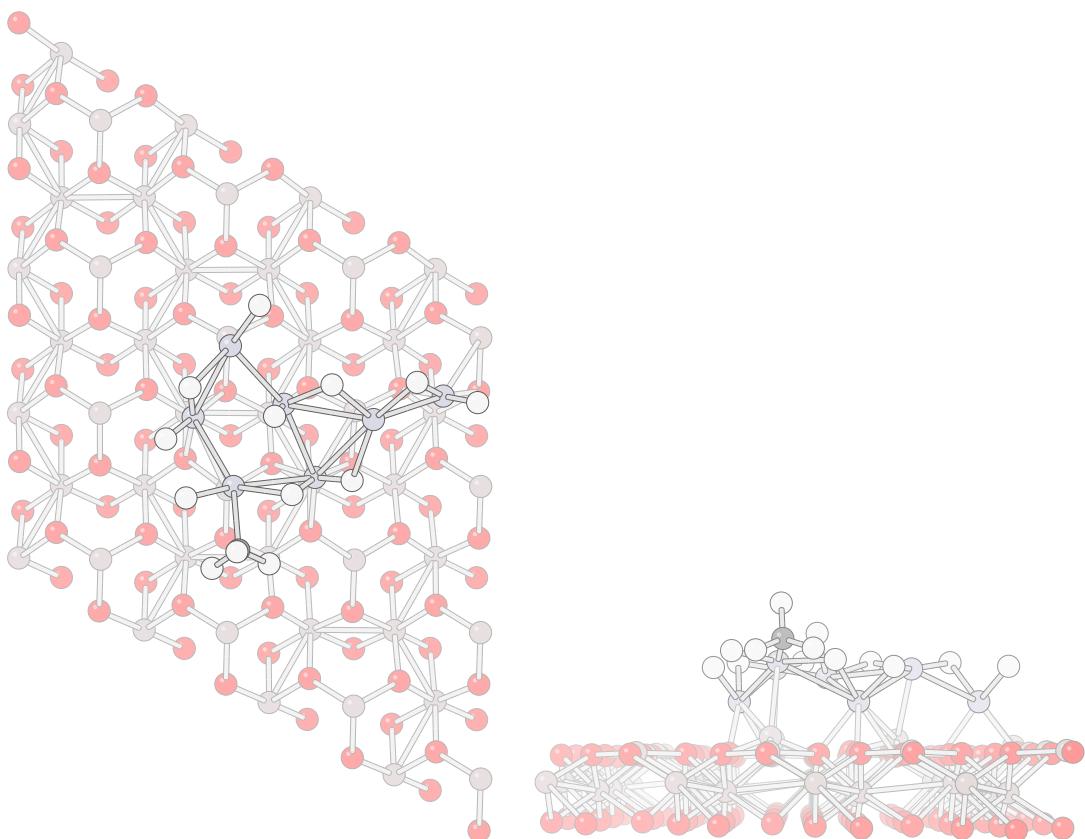
[Relax] Time: 26:50 Step: 103



[47] ~ [35] (d = 0.70) #1.7.191 UNK (doublet)

E = -66.532074 (0.516 eV)

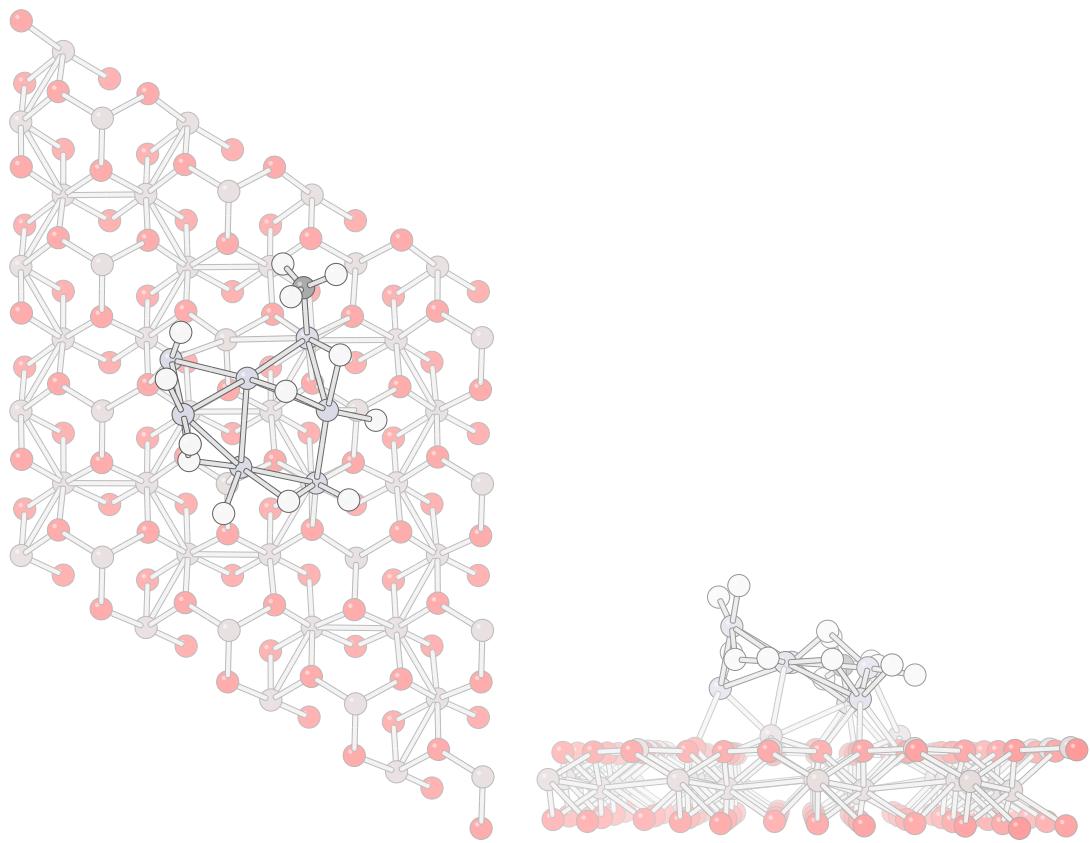
[Relax] Time: 1:25:45 Step: 399



[48] ~ [7] (d = 0.86) #1.8.138 UNK (mixed)

E = -66.531430 (0.534 eV)

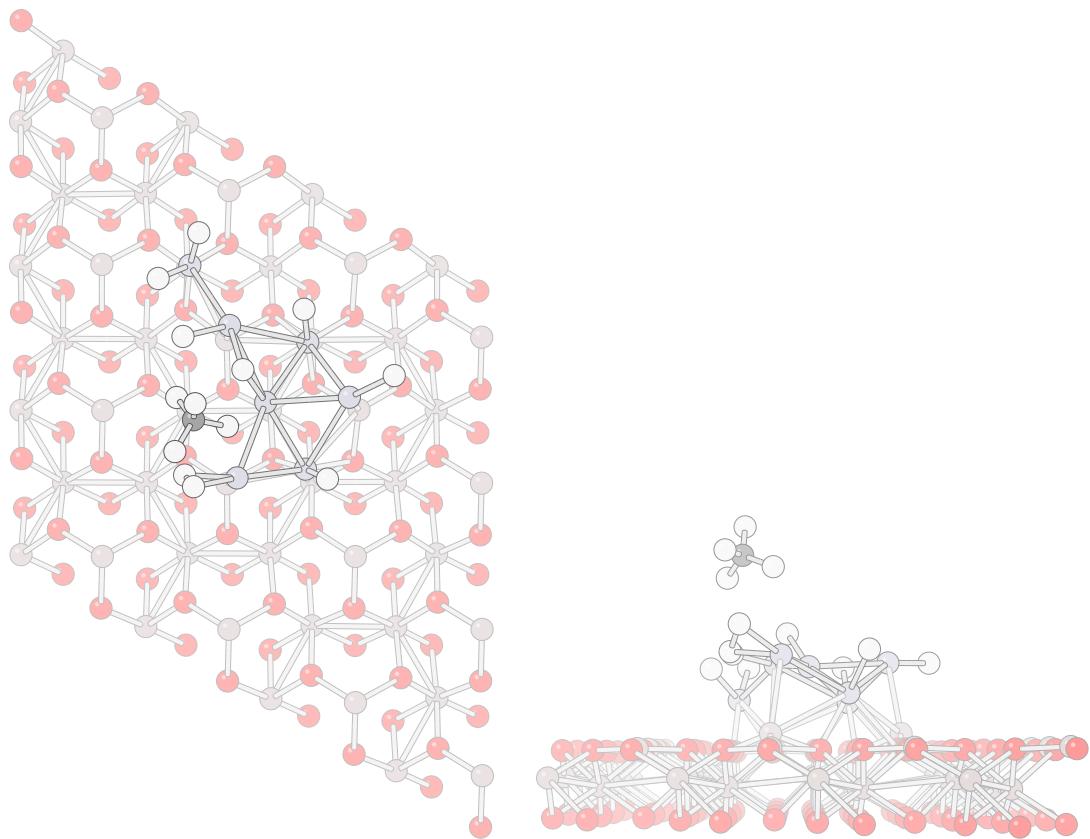
[Relax] Time: 23:13 Step: 99



[49] ~ [8] ($d = 1.59$) #1.7.88 UNK (doublet)

$E = -66.531355$ (0.536 eV)

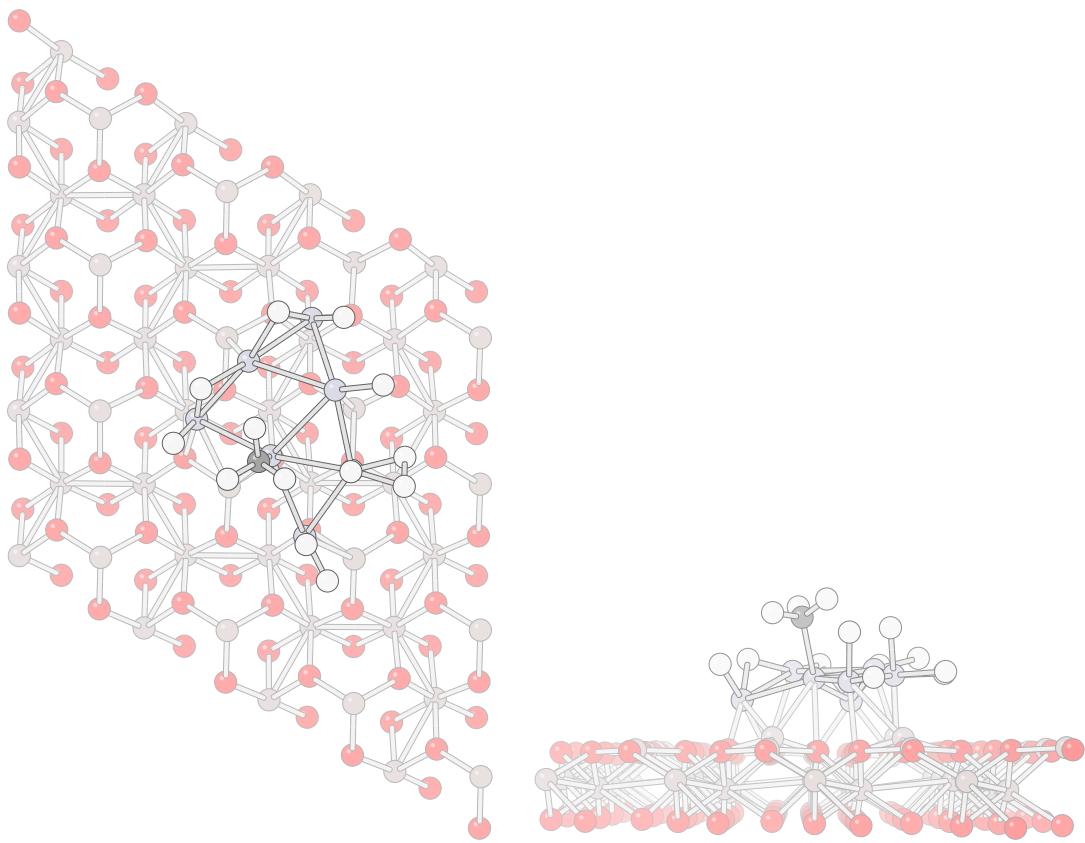
[Relax] Time: 39:47 Step: 164



[50] ~ [13] ($d = 0.70$) #1.0.164 UNK (doublet)

$E = -66.531299$ (0.537 eV)

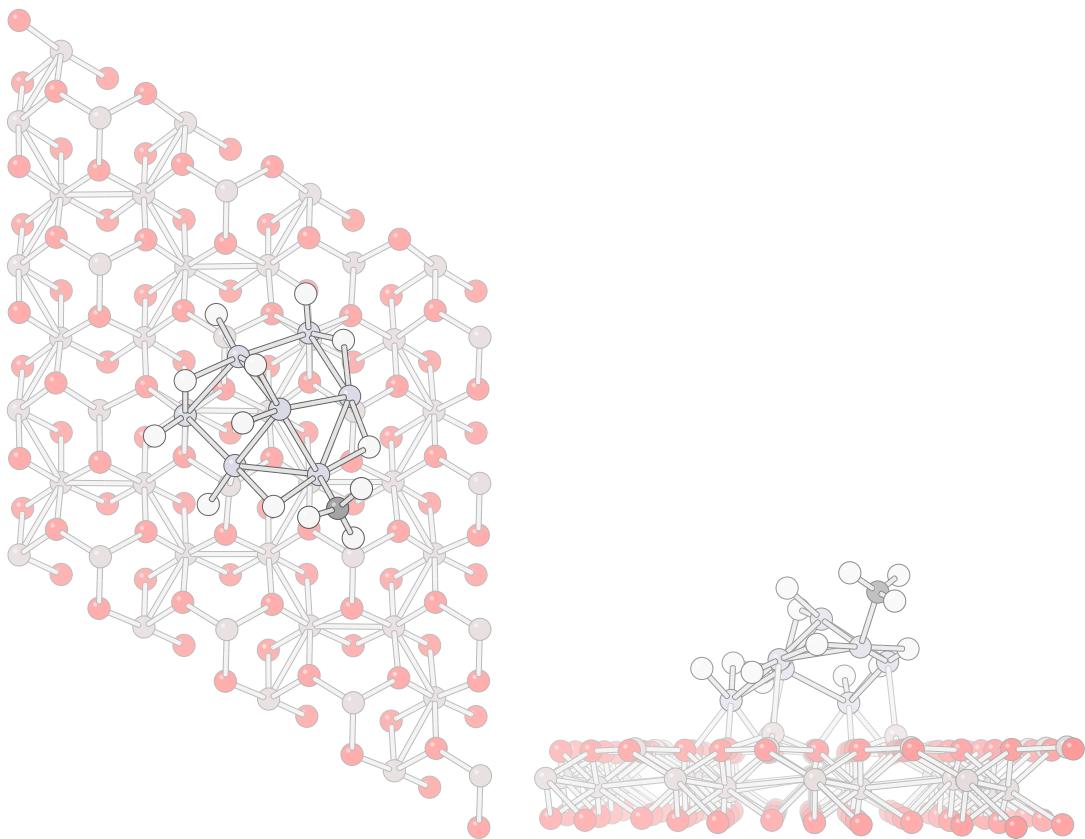
[Relax] Time: 48:56 Step: 171



[51] ~ [27] ($d = 1.05$) #1.3.251 UNK (doublet)

E = -66.531253 (0.538 eV)

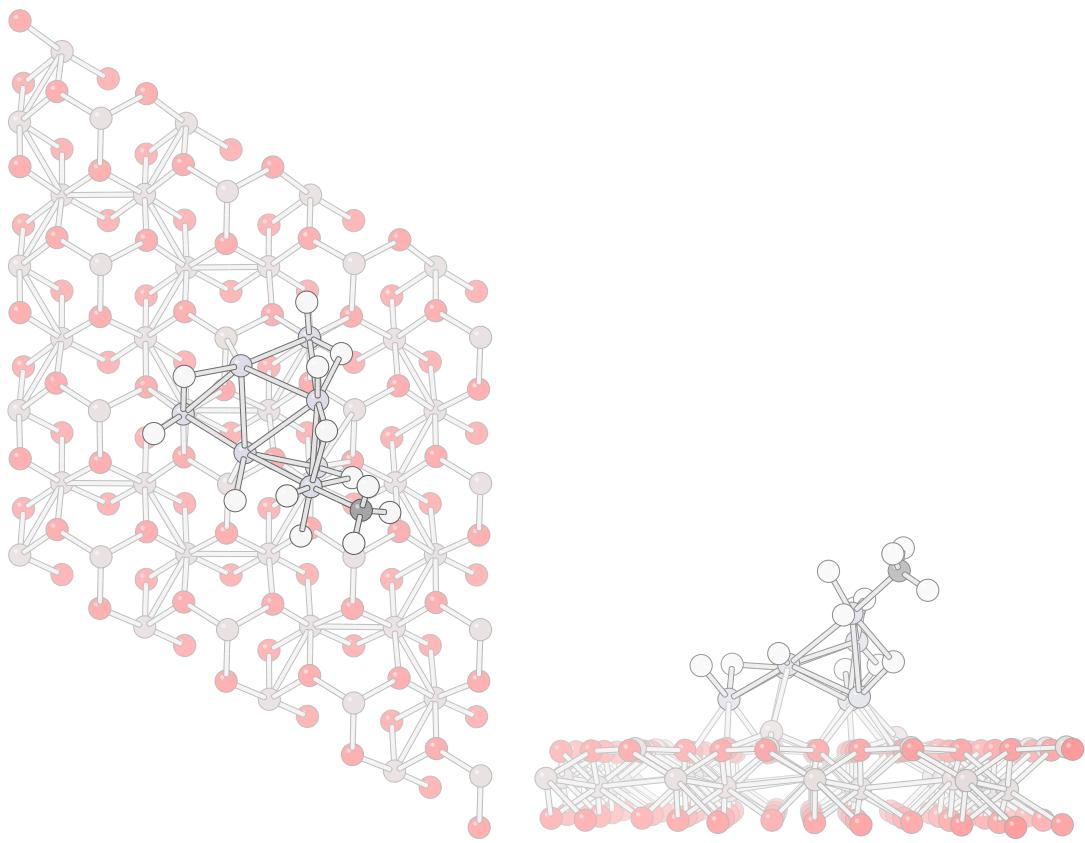
[Relax] Time: 36:03 Step: 153



[52] ~ [41] ($d = 0.52$) #1.9.180 UNK (doublet)

E = -66.531200 (0.540 eV)

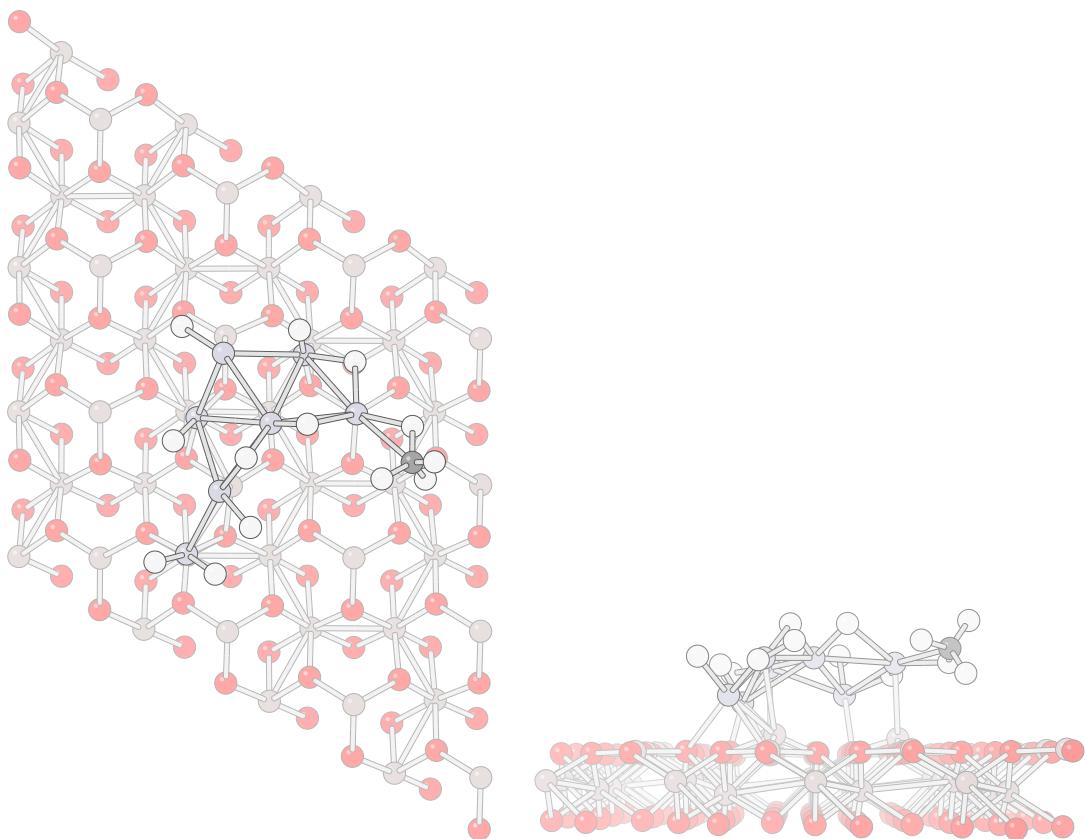
[Relax] Time: 29:09 Step: 107



[53] ~ [49] (d = 1.21) #1.7.251 UNK (doublet)

E = -66.531192 (0.540 eV)

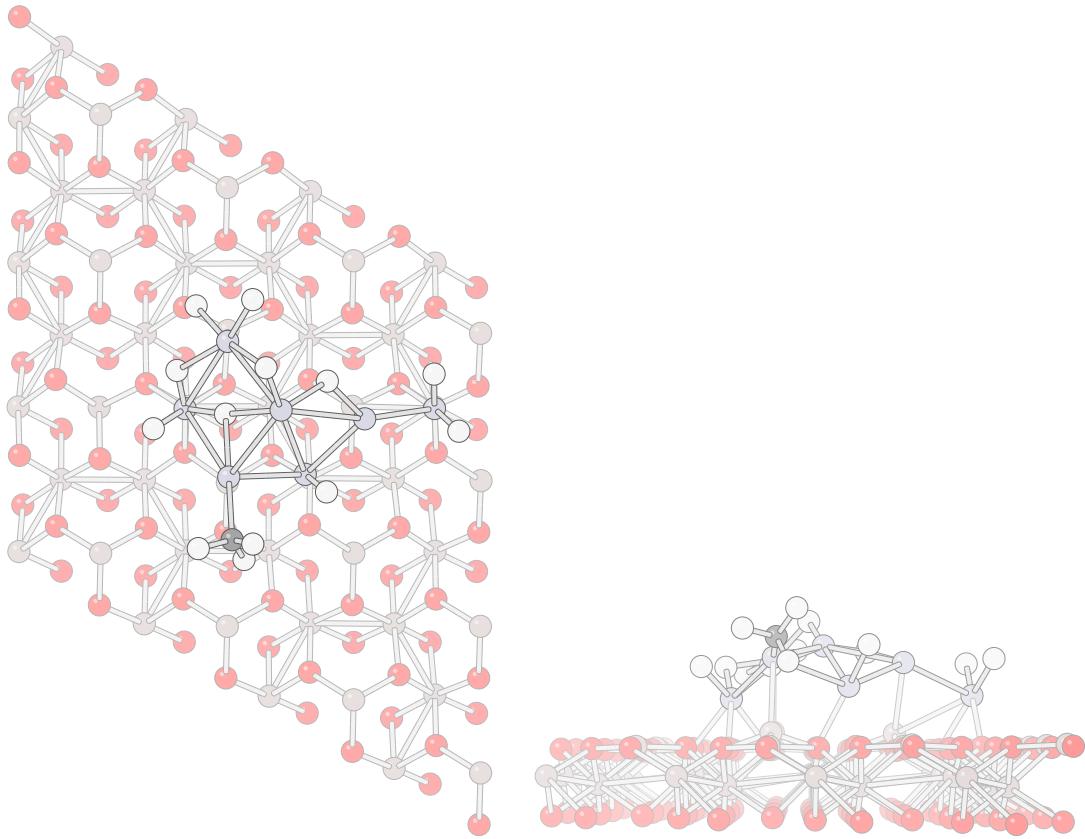
[Relax] Time: 21:48 Step: 109



[54] ~ [2] (d = 0.62) #1.7.184 UNK (doublet)

E = -66.530449 (0.560 eV)

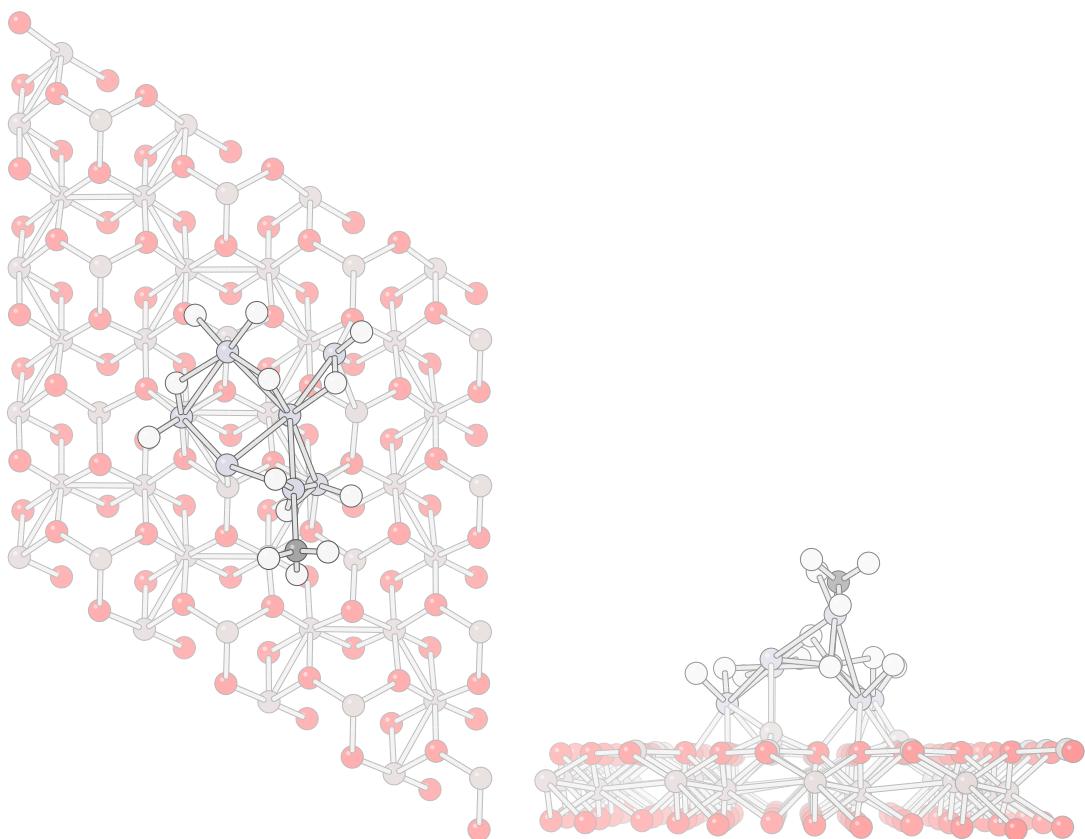
[Relax] Time: 36:32 Step: 139



[55] ~ [30] (d = 1.11) #1.5.260 UNK (doublet)

E = -66.530323 (0.564 eV)

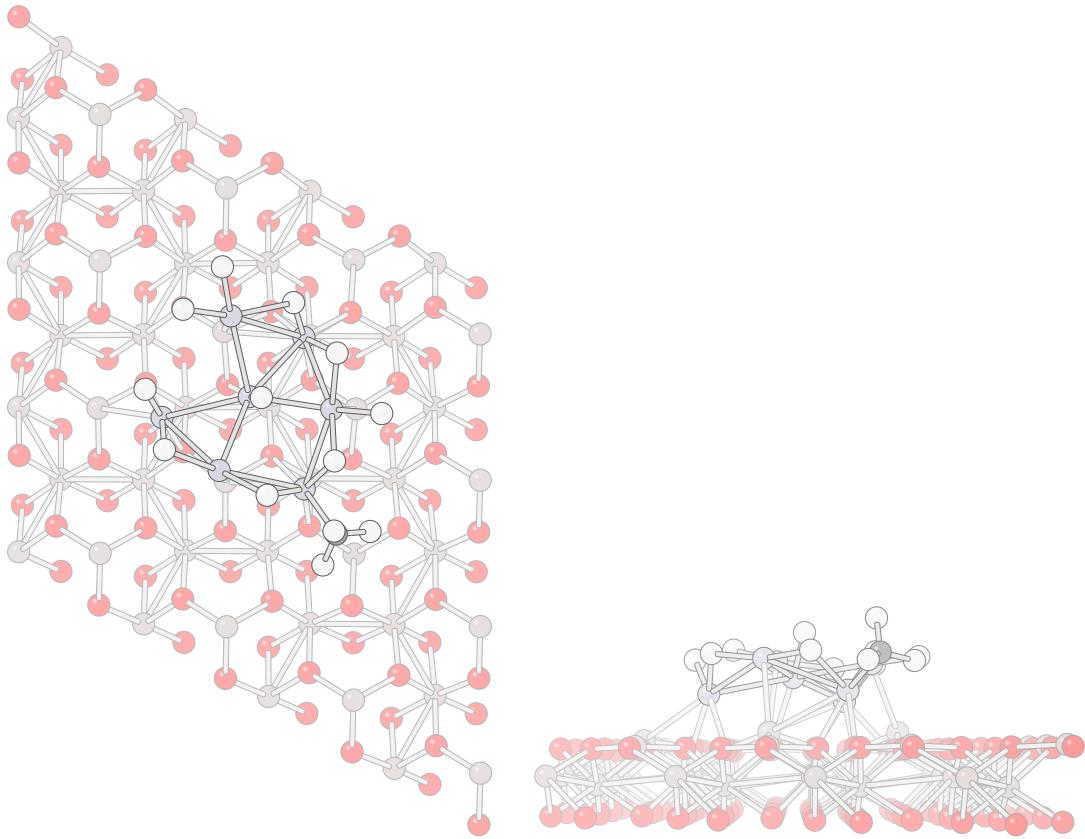
[Relax] Time: 35:30 Step: 129



[56] ~ [43] (d = 1.20) #1.3.206 UNK (mixed)

E = -66.530128 (0.569 eV)

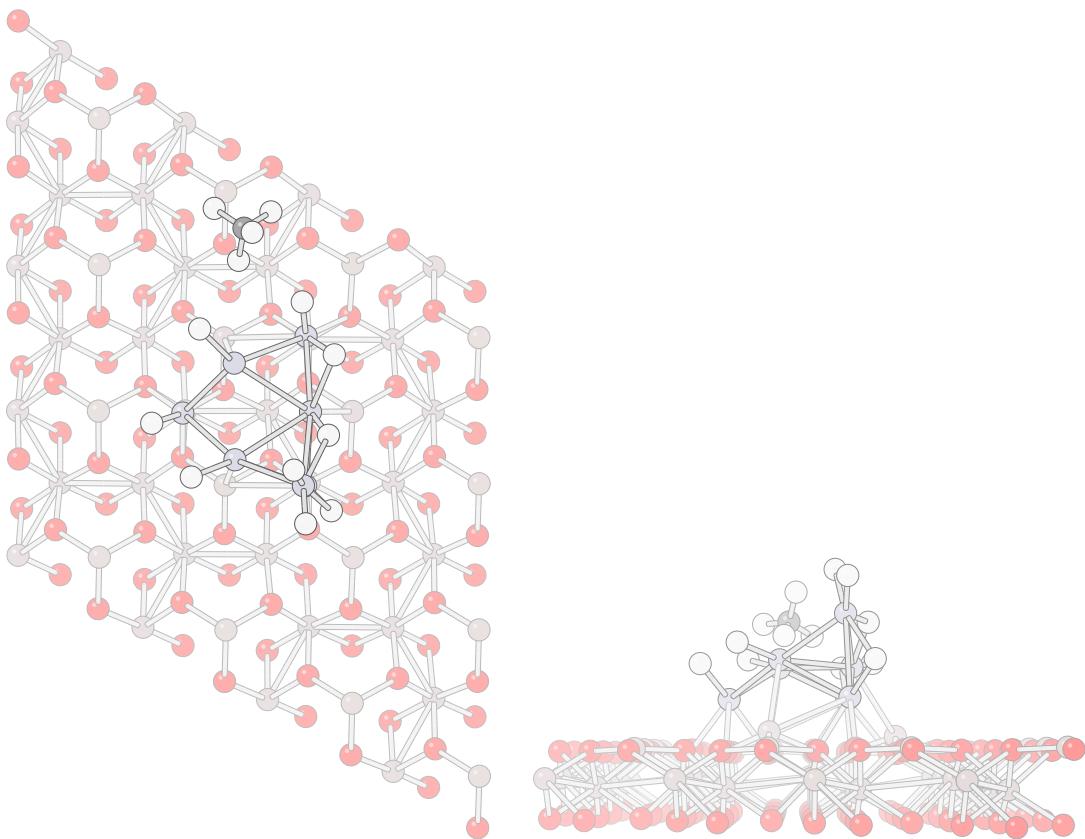
[Relax] Time: 32:52 Step: 130



[57] ~ [38] (d = 1.20) #1.5.67 UNK (mixed)

E = -66.530119 (0.569 eV)

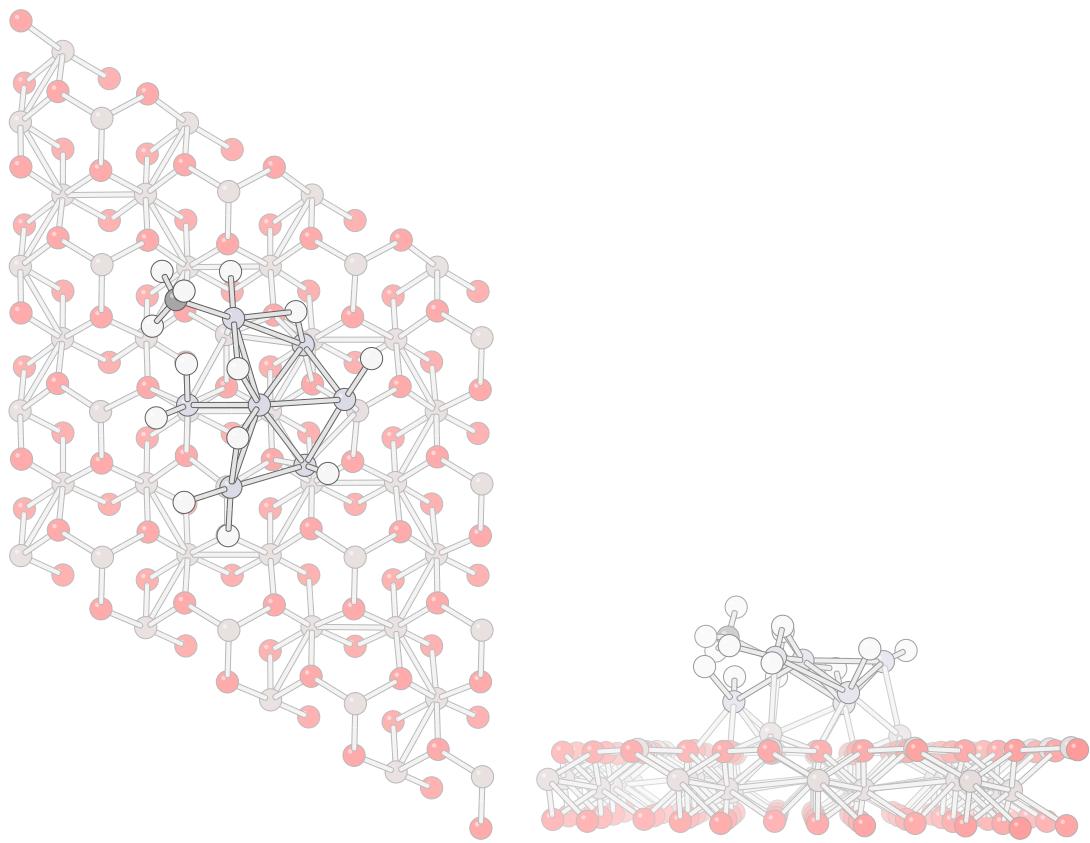
[Relax] Time: 52:46 Step: 157



[58] ~ [14] (d = 0.85) #1.3.162 UNK (doublet)

E = -66.529795 (0.578 eV)

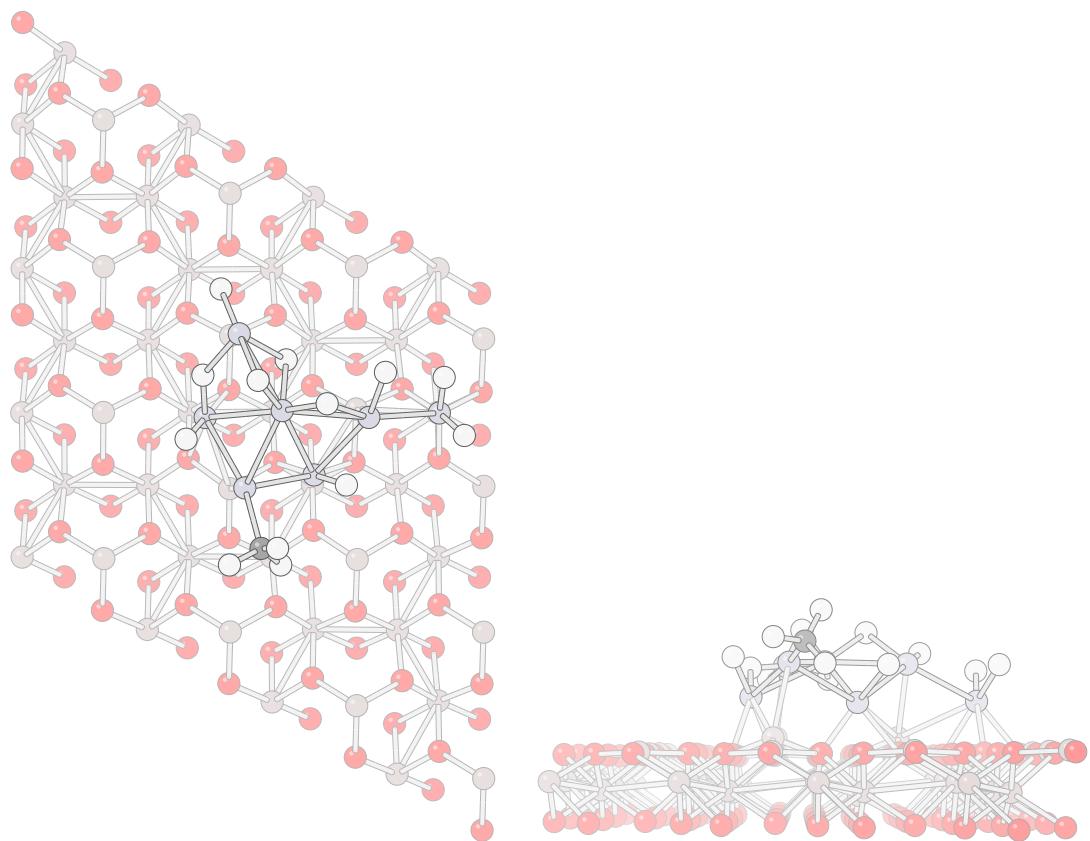
[Relax] Time: 39:13 Step: 169



[59] ~ [8] ($d = 0.31$) #1.7.270 UNK (doublet)

$E = -66.529748$ (0.579 eV)

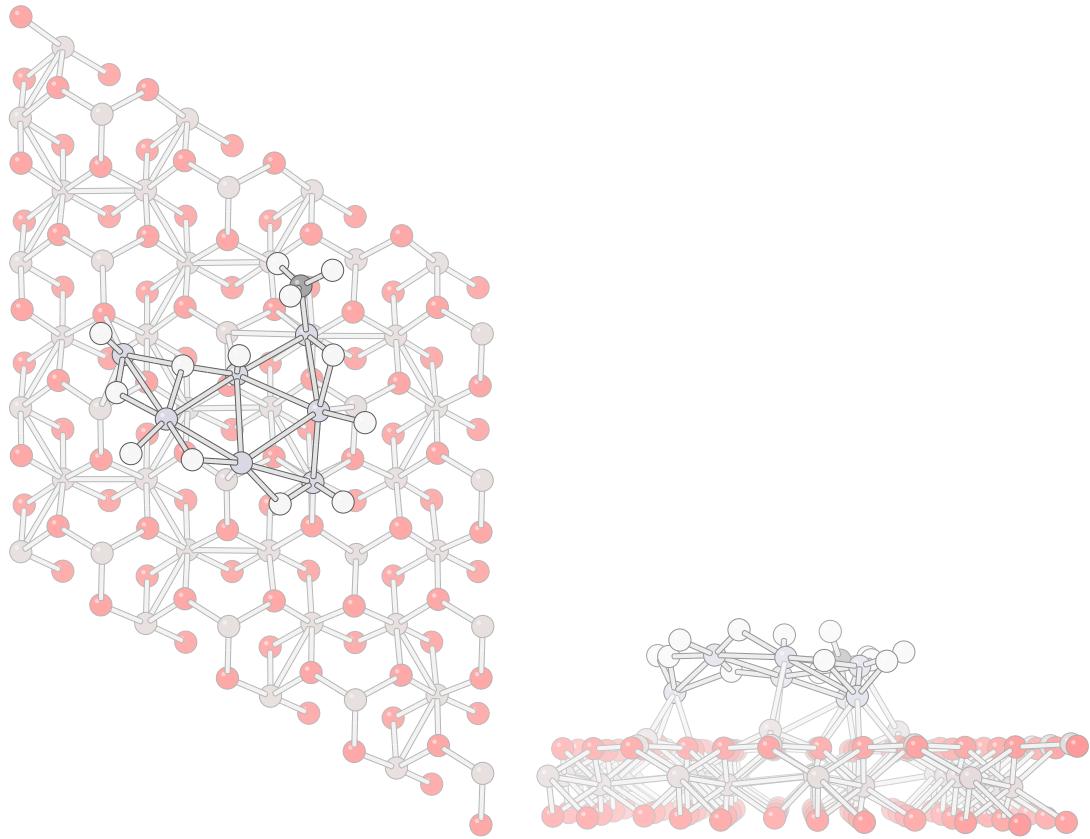
[Relax] Time: 23:29 Step: 119



[60] ~ [18] ($d = 0.47$) #1.8.208 UNK (doublet)

$E = -66.529628$ (0.583 eV)

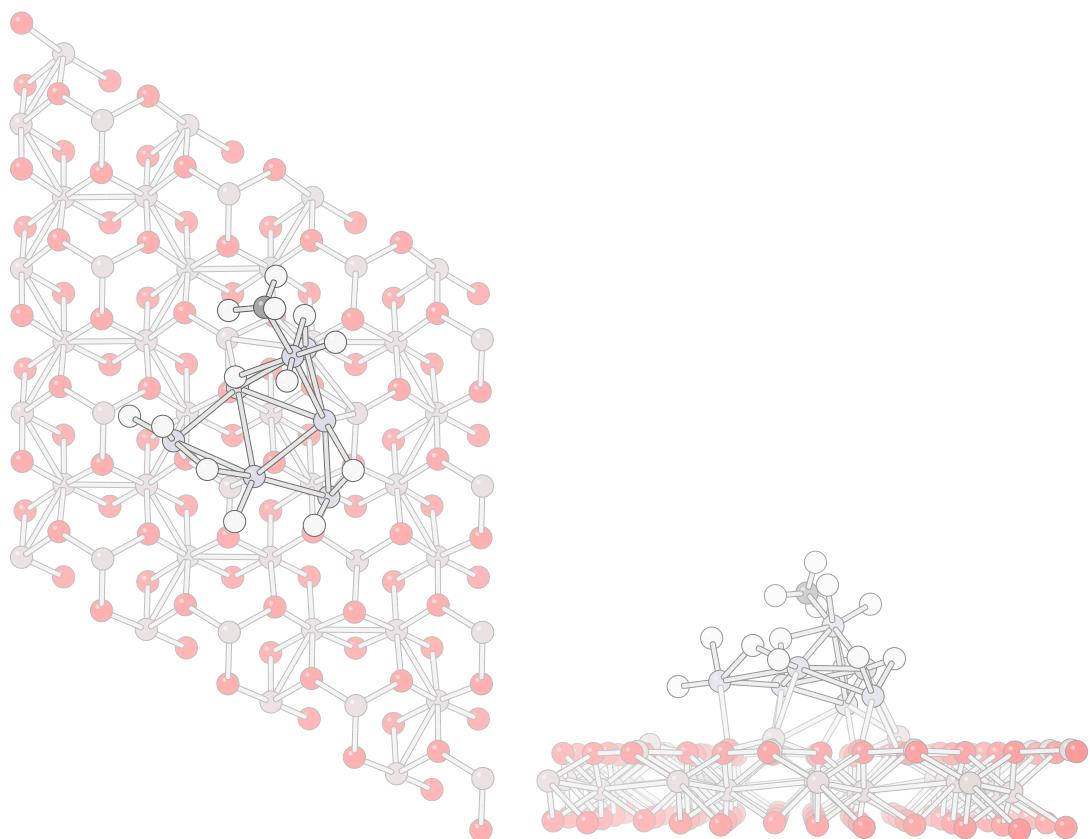
[Relax] Time: 43:35 Step: 198



[61] ~ [30] (d = 0.90) #1.9.76 UNK (mixed)

E = -66.529536 (0.585 eV)

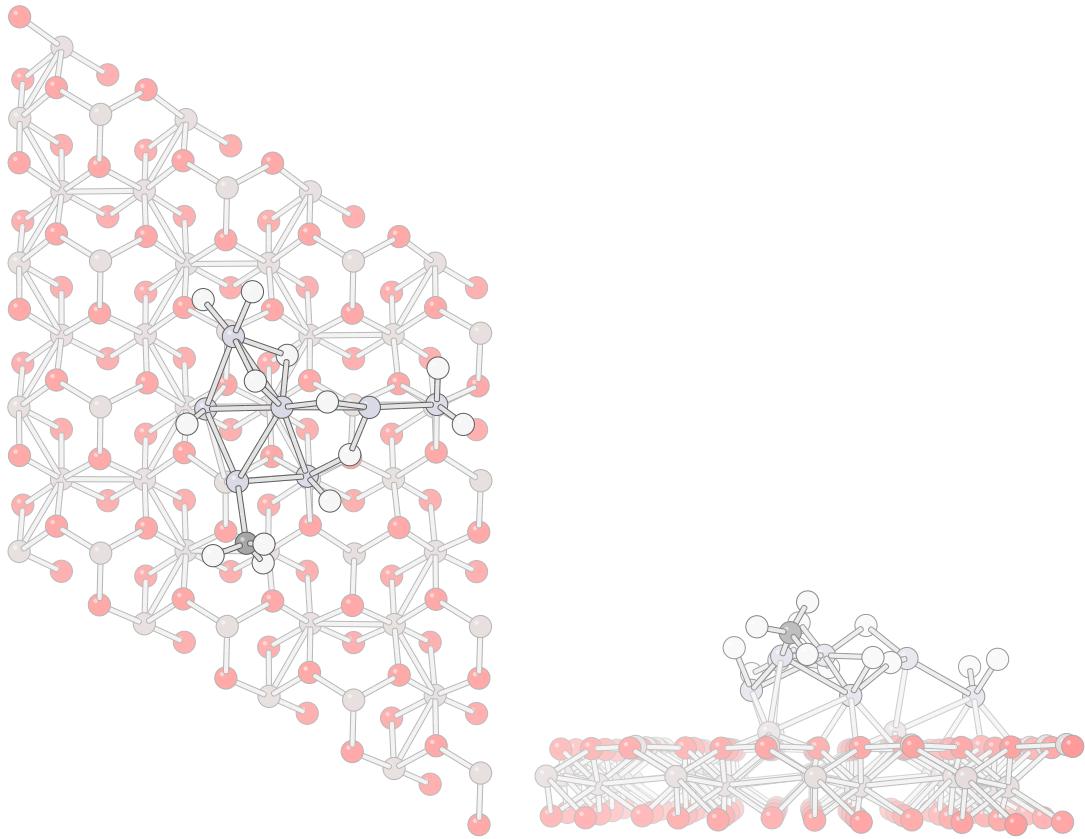
[Relax] Time: 41:03 Step: 179



[62] ~ [8] (d = 0.44) #1.7.73 UNK (doublet)

E = -66.529455 (0.587 eV)

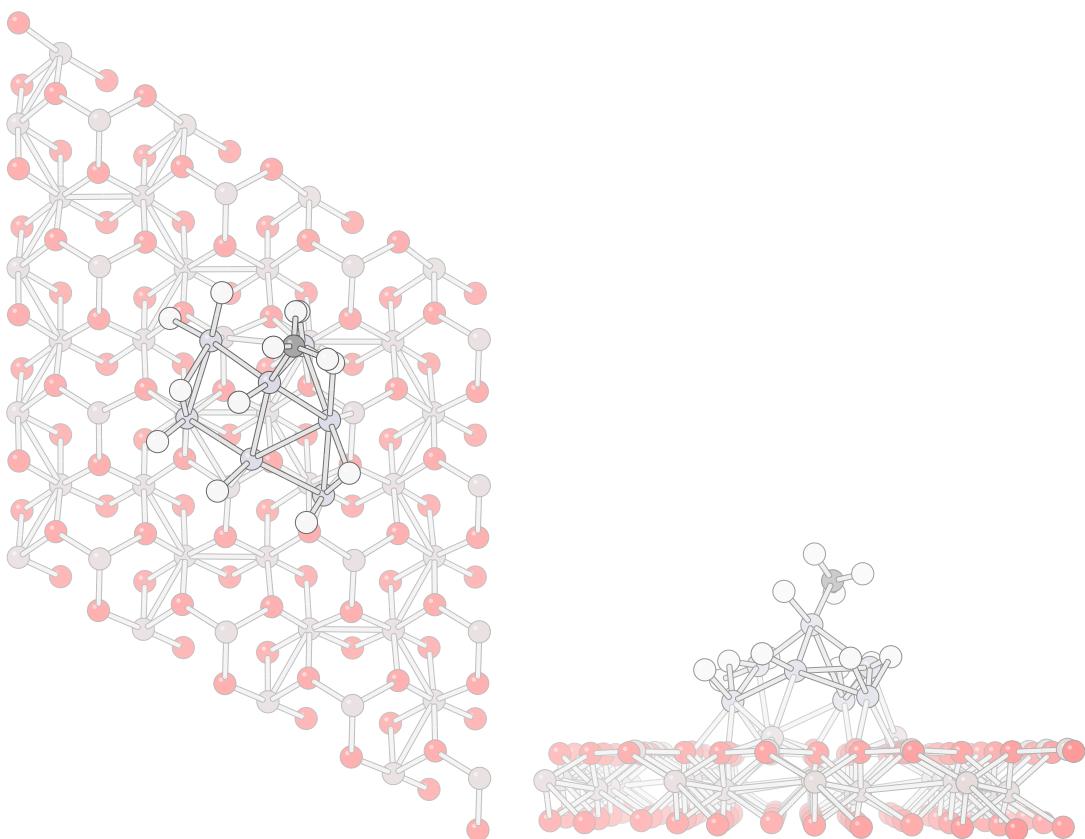
[Relax] Time: 40:15 Step: 148



[63] ~ [33] (d = 0.52) #1.9.209 UNK (doublet)

E = -66.529427 (0.588 eV)

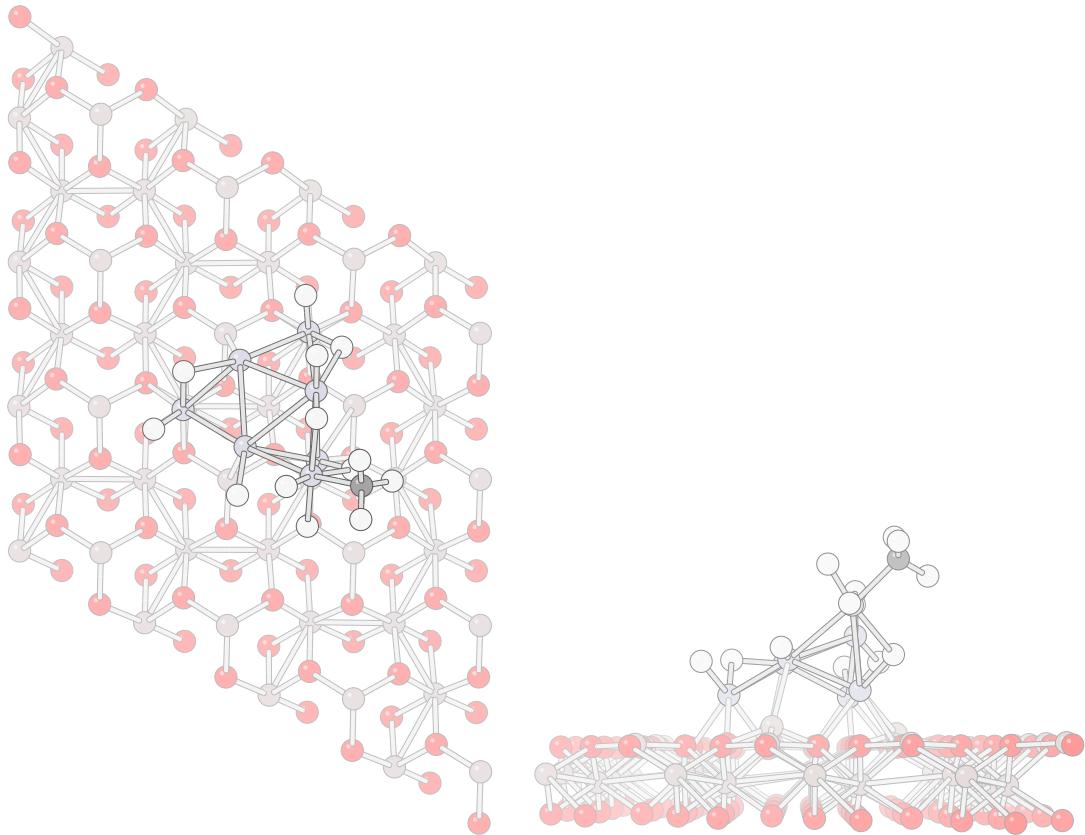
[Relax] Time: 21:23 Step: 95



[64] ~ [52] (d = 0.27) #1.9.158 UNK (doublet)

E = -66.529400 (0.589 eV)

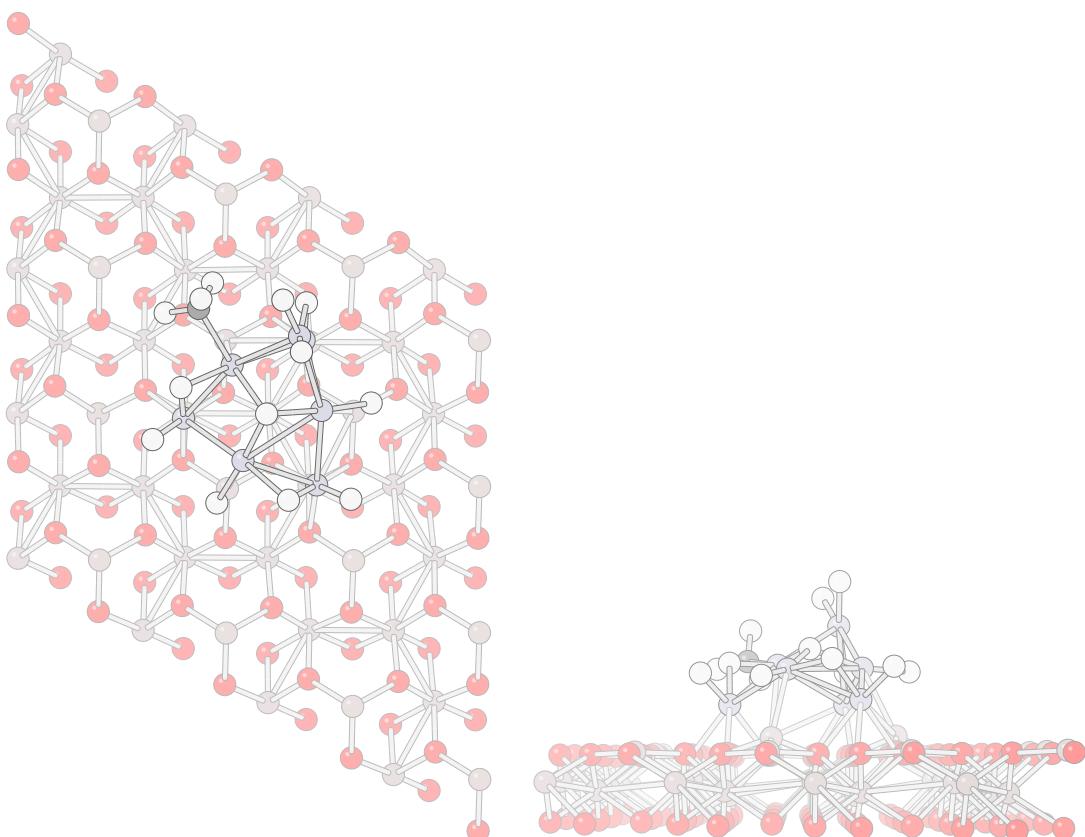
[Relax] Time: 24:15 Step: 100



[65] ~ [21] (d = 0.85) #1.5.299 UNK (doublet)

E = -66.529288 (0.592 eV)

[Relax] Time: 18:19 Step: 67



[66] ~ [11] (d = 0.52) #1.7.202 UNK (doublet)

E = -66.529056 (0.598 eV)

[Relax] Time: 55:48 Step: 246

