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

$[Mn@Si_{12}]^+$: a singlet or triplet ground state?

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Supporting information

1. Comparison with $CrSi_{12}$
2. Comparison of active spaces
3. Analysis of the CASPT2 potential energy surface for $[Mn@Si_{12}]^+$
4. Cartesian coordinates

1 Comparison with $Cr@Si_{12}$.

Table S1 contains a dataset for $Cr@Si_{12}$ which can be compared directly with Table 1 for $[Mn@Si_{12}]^+$. The same set of states has been identified in both cases, but for the chromium system the $^1A_{1g}$ is clearly the ground state, irrespective of the chosen methodology (DFT or CASPT2). This is entirely consistent with all previous work on this molecule.

Table S1. Relative energies, structural data, Mulliken spin densities and values of $<S^2>$ for various states of $Cr@Si_{12}$.

	D_{6h}-symmetric States					C_{2h}-symmetric States		C_s-symmetric states
	$^1A_{1g}$	$^1A_{2u}$	$^3A_{2u}$	$^1E_{2g}$	$^3E_{2g}$	^3A_g	^3B_g	$^3A'$
DFT: BLYP (B3LYP energies in parenthesis)								
Energy / eV	+0.00 (+0.00)	+0.77 (+0.68)	0.76 (+0.83)	+0.89 (+1.13)	+0.69 (+0.70)	+0.59 (+0.31)	+0.58 (+0.30)	+0.58
Cr-Si / Å	2.66 (2.63)	2.67 (2.65)	2.67(2.65)	2.66 (2.64)	2.67 (2.65)	2.61 – 2.76 (2.56 – 2.79)	2.59 – 2.77 (2.55 – 2.79)	2.60 – 2.74
ρ(Cr)	0.00 (0.00)	1.49 (2.29)	1.54(2.02)	1.20 (1.96)	1.99 (2.73)	2.11 (3.00)	1.98 (2.78)	1.98
ρ(Si_{12})	0.00 (0.00)	–1.49 (–2.29)	0.46(–0.02)	-1.20 (–1.96)	0.01 (–0.73)	–0.11 (–1.00)	0.02 (–0.78)	0.02
$<S^2>$	0.00 (0.00)	1.12 (1.64)	2.07(2.24)	§		2.17 (2.65)	2.11 (2.48)	2.12
CASPT2 @ BLYP geometry								
Energy / eV	+0.00	+0.75	+0.75			+0.78	0.72	

2. Comparison of active spaces.

In Table S2 the relative energies for CASPT2 calculations with (10,10) active space are compared to the (10,15) case presented in the main text. The 5 extra orbitals in the (10,15) CAS correspond to the 4d or 'double shell' set that has been shown to be significant for first row transition metals. In this case the energies are rather similar with the exception that the $^1A_{1g}$ state is stabilized relative to the charge transfer states in the larger active space.

Table S2. Relative energies (in eV) for various states of $[Mn@Si_{12}]^+$ obtained with CASPT2 (@BLYP geometry) with different active spaces.

	$^1A_{1g}$	$^1A_{2u}$	$^3A_{2u}$	^3A_g	^3B_g
CAS(10,10) no 4d orbitals	**+0.31**	**+0.06**	**+0.14**	**+0.05**	**0.00**
CAS(10,15)	**+0.17**	**+0.07**	**+0.16**	**+0.06**	**0.00**

3. Analysis of the CASPT2 potential energy surface

In Table S3, the total energies of the various states are presented when either the BLYP or the B3LYP geometry is used. The B3LYP geometries give total energies that lie 0.06-0.13 eV lower in energy, but the key $^1A_{2u} - {}^3B_g$ separation remains essentially unaltered.

Table S3. CASPT2 (10,15) energies (eV) for various states of $[Mn@Si_{12}]^+$ obtained with CASPT2 @BLYP and @B3LYP geometries.

	$^1A_{1g}$	$^1A_{2u}$	$^3A_{2u}$	^3A_g	^3B_g
E (@BLYP geom)	-126096.778	-126096.880	-126096.789	-126096.892	-126096.950
E (@B3LYP geom)	-126096.905	-126096.940	-126096.889	-126096.982	-126097.031

The main structural difference between the B3LYP and BLYP geometries is the Mn-Si bond lengths, which are systematically shorter than in the former by ~0.02 Å. We have therefore systematically varied the Mn-Si distances by increasing/decreasing them in 0.01 Å steps for both $^1A_{2u}$ and ^3B_g geometries (Tables S4 and S5). For D_{6h}-symmetric $^1A_{2u}$ there are only 2 variable (the Mn-Si bond length and the angle to the polar axis) so the geometry was re-optimised for exach Mn-Si distance (B3LYP) before the CASPT2 calculation. For C_{2h}-symmetric ^3B_g the situation is more complicated because there are 4 symmetry distinct Mn-Si distances. We have therefore chosen to decrease all twelve bonds equally from their B3LYP optimized values without further optimisation (Table S5)

Table S4. CASPT2 (10,15) energies (eV) for the $^1A_{2u}$ state at fixed Mn-Si (Å) bond lengths (geometries were optimised with the B3LYP functional).

d(Mn-Si), Å	CASPT2 energy, eV
2.61	-126097.019
2.62	-126097.026
2.625	-126097.024
2.63	-126097.019
2.64	-126096.999
2.65	-126096.967
2.66	-126096.920
2.67	-126096.862
2.68	-126096.795
2.69	-126096.717

Table S5. CASPT2 (10,15) energies (eV) for the ^3B_g state at fixed Mn-Si (Å) bond lengths (Mn-Si bondlengths were modified (each by 0.01 Å at a time) for the geometry optimised with the B3LYP functional).

d(Mn-$Si_{1/12}$), Å	d(Mn-$Si_{4/5/8/9}$), Å	d(Mn-$Si_{2/3/10/11}$), Å	d(Mn-$Si_{6/7}$), Å	CASPT2 energy, eV
2.51	2.56	2.69	2.56	-126097.035
2.52	2.57	2.70	2.57	-126097.072
2.53	2.58	2.71	2.58	-126097.093
2.54	2.59	2.72	2.59	-126097.100
2.55	2.60	2.73	2.60	-126097.093
2.56	2.61	2.74	2.61	-126097.071
2.57	2.62	2.75	2.62	-126097.037

The data in Tables S4 an S5 are summarised schematically in Figure S1 (schematically because the coordinate that describes the distortion from the minimum is not easily defined). The BLYP geometries lie further from the CASPT2 minimum than B3LYP, but the surfaces lie parallel and so the key conclusion, that the triplet lies below the singlet, is robust to these changes.

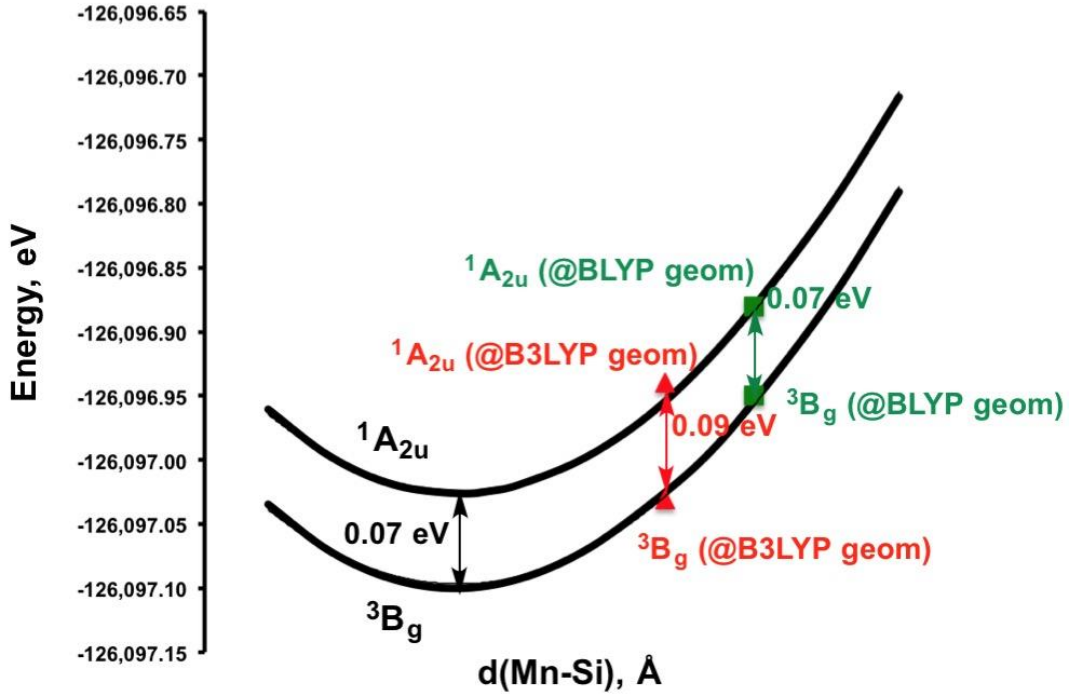

Figure S1. Schematic representation of the potential energy curve for the $^1A_{2u}$ and ^3B_g states of $[Mn@Si_{12}]^+$ obtained with CASPT2 (10,15). All the data used can be found in Table S1, Table S2 and Table S3.

4. Optimised Cartesian coordinates for all states.

Table S6. Cartesian coordinates and total energies of all stationary points for $[Mn@Si_{12}]^+$

BLYP	B3LYP
$^1A_{1g}$, BLYP functional, E=-49.00647681 eV	**$^1A_{1g}$, B3LYP functional, E=-64.15041444 eV**
1.Si -2.367662 0.000000 1.198187	1.Si -2.343262 0.000000 1.191430
2.Si -1.183831 2.050455 1.198187	2.Si -1.171631 2.029325 1.191430
3.Si -1.183831 -2.050455 1.198187	3.Si -1.171631 -2.029325 1.191430
4.Si 1.183831 2.050455 1.198187	4.Si 1.171631 2.029325 1.191430
5.Si 1.183831 -2.050455 1.198187	5.Si 1.171631 -2.029325 1.191430
6.Si 2.367662 0.000000 1.198187	6.Si 2.343262 0.000000 1.191430
7.Si -2.367662 0.000000 -1.198187	7.Si -2.343262 0.000000 -1.191430
8.Si -1.183831 2.050455 -1.198187	8.Si -1.171631 2.029325 -1.191430
9.Si -1.183831 -2.050455 -1.198187	9.Si -1.171631 -2.029325 -1.191430
10.Si 1.183831 2.050455 -1.198187	10.Si 1.171631 2.029325 -1.191430
11.Si 1.183831 -2.050455 -1.198187	11.Si 1.171631 -2.029325 -1.191430
12.Si 2.367662 0.000000 -1.198187	12.Si 2.343262 0.000000 -1.191430
13.Mn 0.000000 0.000000 0.000000	13.Mn 0.000000 0.000000 0.000000
$^1A_{2u}$, BLYP functional, E=-49.02887420 eV	**$^1A_{2u}$, B3LYP functional, E= -64.41585116 eV**
1.Si -2.386474 0.000000 1.190175	1.Si -2.376906 0.000000 1.186682
2.Si -1.193237 2.066747 1.190175	2.Si -1.188453 2.058461 1.186682
3.Si -1.193237 -2.066747 1.190175	3.Si -1.188453 -2.058461 1.186682
4.Si 1.193237 2.066747 1.190175	4.Si 1.188453 2.058461 1.186682
5.Si 1.193237 -2.066747 1.190175	5.Si 1.188453 -2.058461 1.186682
6.Si 2.386474 0.000000 1.190175	6.Si 2.376906 0.000000 1.186682
7.Si -2.386474 0.000000 -1.190175	7.Si -2.376906 0.000000 -1.186682
8.Si -1.193237 2.066747 -1.190175	8.Si -1.188453 2.058461 -1.186682
9.Si -1.193237 -2.066747 -1.190175	9.Si -1.188453 -2.058461 -1.186682
10.Si 1.193237 2.066747 -1.190175	10.Si 1.188453 2.058461 -1.186682
11.Si 1.193237 -2.066747 -1.190175	11.Si 1.188453 -2.058461 -1.186682
12.Si 2.386474 0.000000 -1.190175	12.Si 2.376906 0.000000 -1.186682
13.Mn 0.000000 0.000000 0.000000	13.Mn 0.000000 0.000000 0.000000
$^3A_{2u}$, BLYP functional, E=-49.00481475 eV	**$^3A_{2u}$, B3LYP functional, E=-64.13292363 eV**
1.Si -2.384155 0.000000 1.189342	1.Si -2.368739 0.000000 1.183764
2.Si -1.192078 2.064739 1.189342	2.Si -1.184369 2.051388 1.183764
3.Si -1.192078 -2.064739 1.189342	3.Si -1.184369 -2.051388 1.183764
4.Si 1.192078 2.064739 1.189342	4.Si 1.184369 2.051388 1.183764
5.Si 1.192078 -2.064739 1.189342	5.Si 1.184369 -2.051388 1.183764
6.Si 2.384155 0.000000 1.189342	6.Si 2.368739 0.000000 1.183764
7.Si -2.384155 0.000000 -1.189342	7.Si -2.368739 0.000000 -1.183764

8.Si -1.192078 2.064739 -1.189342 9.Si -1.192078 -2.064739 -1.189342 10.Si 1.192078 2.064739 -1.189342 11.Si 1.192078 -2.064739 -1.189342 12.Si 2.384155 0.000000 -1.189342 13.Mn 0.000000 0.000000 0.000000	8.Si -1.184369 2.051388 -1.183764 9.Si -1.184369 -2.051388 -1.183764 10.Si 1.184369 2.051388 -1.183764 11.Si 1.184369 -2.051388 -1.183764 12.Si 2.368739 0.000000 -1.183764 13.Mn 0.000000 0.000000 0.000000
$^{1}E_{2g}$, BLYP functional, E=-48.78749984 eV 1.Si -2.354738 0.000000 1.219680 2.Si -1.177369 2.039263 1.219680 3.Si -1.177369 -2.039263 1.219680 4.Si 1.177369 2.039263 1.219680 5.Si 1.177369 -2.039263 1.219680 6.Si 2.354738 0.000000 1.219680 7.Si -2.354738 0.000000 -1.219680 8.Si -1.177369 2.039263 -1.219680 9.Si -1.177369 -2.039263 -1.219680 10.Si 1.177369 2.039263 -1.219680 11.Si 1.177369 -2.039263 -1.219680 12.Si 2.354738 0.000000 -1.219680 13.Mn 0.000000 0.000000 0.000000	**$^{1}E_{2g}$, B3LYP functional, E=-63.78203179 eV** 1.Si -2.339345 0.000000 1.220604 2.Si -1.169673 2.025933 1.220604 3.Si -1.169673 -2.025933 1.220604 4.Si 1.169673 2.025933 1.220604 5.Si 1.169673 -2.025933 1.220604 6.Si 2.339345 0.000000 1.220604 7.Si -2.339345 0.000000 -1.220604 8.Si -1.169673 2.025933 -1.220604 9.Si -1.169673 -2.025933 -1.220604 10.Si 1.169673 2.025933 -1.220604 11.Si 1.169673 -2.025933 -1.220604 12.Si 2.339345 0.000000 -1.220604 13.Mn 0.000000 0.000000 0.000000
$^{3}E_{2g}$, BLYP functional, E=-48.98262524 eV 1.Si -2.371665 0.000000 1.212329 2.Si -1.185832 2.053922 1.212329 3.Si -1.185832 -2.053922 1.212329 4.Si 1.185832 2.053922 1.212329 5.Si 1.185832 -2.053922 1.212329 6.Si 2.371665 0.000000 1.212329 7.Si -2.371665 0.000000 -1.212329 8.Si -1.185832 2.053922 -1.212329 9.Si -1.185832 -2.053922 -1.212329 10.Si 1.185832 2.053922 -1.212329 11.Si 1.185832 -2.053922 -1.212329 12.Si 2.371665 0.000000 -1.212329 13.Mn 0.000000 0.000000 0.000000	**$^{3}E_{2g}$, B3LYP functional, E=-64.24144173 eV** 1.Si -2.364059 0.000000 1.207857 2.Si -1.182029 2.047335 1.207857 3.Si -1.182029 -2.047335 1.207857 4.Si 1.182029 2.047335 1.207857 5.Si 1.182029 -2.047335 1.207857 6.Si 2.364059 0.000000 1.207857 7.Si -2.364059 0.000000 -1.207857 8.Si -1.182029 2.047335 -1.207857 9.Si -1.182029 -2.047335 -1.207857 10.Si 1.182029 2.047335 -1.207857 11.Si 1.182029 -2.047335 -1.207857 12.Si 2.364059 0.000000 -1.207857 13.Mn 0.000000 0.000000 0.000000
$^{3}A_{g}$, BLYP functional, E=-49.09722408 eV 1.Si -1.259520 -2.451849 0.000000 2.Si -1.199046 -1.181196 -1.988375 3.Si -1.199046 -1.181196 1.988375 4.Si -1.196898 1.222106 -2.040785 5.Si -1.196898 1.222106 2.040785	**$^{3}A_{g}$, B3LYP functional, E=-64.60396832 eV** 1.Si -1.265486 -2.424070 0.000000 2.Si -1.189743 -1.182308 -1.989596 3.Si -1.189743 -1.182308 1.989596 4.Si -1.201710 1.209192 -2.032188 5.Si -1.201710 1.209192 2.032188

6.Si -1.228362 2.404340 0.000000 7.Si 1.228362 -2.404340 0.000000 8.Si 1.196898 -1.222106 -2.040785 9.Si 1.196898 -1.222106 2.040785 10.Si 1.199046 1.181196 -1.988375 11.Si 1.199046 1.181196 1.988375 12.Si 1.259520 2.451849 0.000000 13.Mn 0.000000 0.000000 0.000000	6.Si -1.196711 2.388743 0.000000 7.Si 1.196711 -2.388743 0.000000 8.Si 1.201710 -1.209192 -2.032188 9.Si 1.201710 -1.209192 2.032188 10.Si 1.189743 1.182308 -1.989596 11.Si 1.189743 1.182308 1.989596 12.Si 1.265486 2.424070 0.000000 13.Mn 0.000000 0.000000 0.000000
^3B_g, BLYP functional, E= -49.09477400 eV 1.Si -1.196356 -2.281646 0.000000 2.Si -1.253198 -1.222433 -2.134118 3.Si -1.253198 -1.222433 2.134118 4.Si -1.196210 1.126006 -2.068813 5.Si -1.196210 1.126006 2.068813 6.Si -1.173736 2.338749 0.000000 7.Si 1.173736 -2.338749 0.000000 8.Si 1.196210 -1.126006 -2.068813 9.Si 1.196210 -1.126006 2.068813 10.Si 1.253198 1.222433 -2.134118 11.Si 1.253198 1.222433 2.134118 12.Si 1.196356 2.281646 0.000000 13.Mn 0.000000 0.000000 0.000000	**^3B_g, BLYP functional, E=-64.62391273 eV** 1.Si -1.177619 -2.287221 0.000000 2.Si -1.264063 -1.221850 -2.115539 3.Si -1.264063 -1.221850 2.115539 4.Si -1.158600 1.123381 -2.065017 5.Si -1.158600 1.123381 2.065017 6.Si -1.195125 2.335255 0.000000 7.Si 1.195125 -2.335255 0.000000 8.Si 1.158600 -1.123381 -2.065017 9.Si 1.158600 -1.123381 2.065017 10.Si 1.264063 1.221850 -2.115539 11.Si 1.264063 1.221850 2.115539 12.Si 1.177619 2.287221 0.000000 13.Mn 0.000000 0.000000 0.000000
3A', BLYP functional, E=-49.10034321 eV 1.Si 0.060904 -1.226727 -2.367326 2.Si -1.991788 -1.337614 -1.192696 3.Si 2.110554 -1.053838 -1.195820 4.Si -1.991788 -1.337614 1.192696 5.Si 2.110554 -1.053838 1.195820 6.Si 0.060904 -1.226727 2.367326 7.Si -0.057076 1.233383 -2.495949 8.Si -2.029838 1.053687 -1.218596 9.Si 1.911870 1.331327 -1.196076 10.Si -2.029838 1.053687 1.218596 11.Si 1.911870 1.331327 1.196076 12.Si -0.057076 1.233383 2.495949 13.Mn -0.004713 -0.000227 0.000000	

Table 4S. Cartesian coordinates and total energies of all stationary points for Cr@Si_{12}

$^1A_{1g}$, BLYP functional, E=-55.60827270 eV	**$^1A_{1g}$, B3LYP functional, E=-70.73135257 eV**

1.Si 2.050585 1.183906 1.203427 2.Si 2.050585 -1.183906 1.203427 3.Si 0.000000 2.367812 1.203427 4.Si 0.000000 -2.367812 1.203427 5.Si -2.050585 1.183906 1.203427 6.Si -2.050585 -1.183906 1.203427 7.Si 2.050585 1.183906 -1.203427 8.Si 2.050585 -1.183906 -1.203427 9.Si 0.000000 2.367812 -1.203427 10.Si 0.000000 -2.367812 -1.203427 11.Si -2.050585 1.183906 -1.203427 12.Si -2.050585 -1.183906 -1.203427 13.Cr 0.000000 0.000000 0.000000	1.Si 2.029794 1.171902 1.194621 2.Si 2.029794 -1.171902 1.194621 3.Si 0.000000 2.343804 1.194621 4.Si 0.000000 -2.343804 1.194621 5.Si -2.029794 1.171902 1.194621 6.Si -2.029794 -1.171902 1.194621 7.Si 2.029794 1.171902 -1.194621 8.Si 2.029794 -1.171902 -1.194621 9.Si 0.000000 2.343804 -1.194621 10.Si 0.000000 -2.343804 -1.194621 11.Si -2.029794 1.171902 -1.194621 12.Si -2.029794 -1.171902 -1.194621 13.Cr 0.000000 0.000000 0.000000
$^1A_{2u}$, BLYP functional, E=-54.83800104 eV 1.Si 2.068394 1.194188 1.193794 2.Si 2.068394 -1.194188 1.193794 3.Si 0.000000 2.388376 1.193794 4.Si 0.000000 -2.388376 1.193794 5.Si -2.068394 1.194188 1.193794 6.Si -2.068394 -1.194188 1.193794 7.Si 2.068394 1.194188 -1.193794 8.Si 2.068394 -1.194188 -1.193794 9.Si 0.000000 2.388376 -1.193794 10.Si 0.000000 -2.388376 -1.193794 11.Si -2.068394 1.194188 -1.193794 12.Si -2.068394 -1.194188 -1.193794 13.Cr 0.000000 0.000000 0.000000	**$^1A_{2u}$, B3LYP functional, E=-70.04700419** 1.Si 2.054883 1.186387 1.188339 2.Si 2.054883 -1.186387 1.188339 3.Si 0.000000 2.372774 1.188339 4.Si 0.000000 -2.372774 1.188339 5.Si -2.054883 1.186387 1.188339 6.Si -2.054883 -1.186387 1.188339 7.Si 2.054883 1.186387 -1.188339 8.Si 2.054883 -1.186387 -1.188339 9.Si 0.000000 2.372774 -1.188339 10.Si 0.000000 -2.372774 -1.188339 11.Si -2.054883 1.186387 -1.188339 12.Si -2.054883 -1.186387 -1.188339 13.Cr 0.000000 0.000000 0.000000
$^3A_{2u}$, BLYP functional, E= -54.83900670 eV 1.Si 2.067070 1.193423 1.193326 2.Si 2.067070 -1.193423 1.193326 3.Si 0.000000 2.386847 1.193326 4.Si 0.000000 -2.386847 1.193326 5.Si -2.067070 1.193423 1.193326 6.Si -2.067070 -1.193423 1.193326 7.Si 2.067070 1.193423 -1.193326 8.Si 2.067070 -1.193423 -1.193326 9.Si 0.000000 2.386847 -1.193326 10.Si 0.000000 -2.386847 -1.193326 11.Si -2.067070 1.193423 -1.193326 12.Si -2.067070 -1.193423 -1.193326 13.Cr 0.000000 0.000000 0.000000	**$^3A_{2u}$, B3LYP functional, E=-69.89744007 eV** 1.Si 2.049728 1.183411 1.185730 2.Si 2.049728 -1.183411 1.185730 3.Si 0.000000 2.366822 1.185730 4.Si 0.000000 -2.366822 1.185730 5.Si -2.049728 1.183411 1.185730 6.Si -2.049728 -1.183411 1.185730 7.Si 2.049728 1.183411 -1.185730 8.Si 2.049728 -1.183411 -1.185730 9.Si 0.000000 2.366822 -1.185730 10.Si 0.000000 -2.366822 -1.185730 11.Si -2.049728 1.183411 -1.185730 12.Si -2.049728 -1.183411 -1.185730 13.Cr 0.000000 0.000000 0.000000

$^1E_{2g}$, BLYP functional, E=-54.71144388 eV	**$^1E_{2g}$, B3LYP functional, E=-69.60198913 eV**
1.Si 2.048893 1.182929 1.219683	1.Si 2.029669 1.171830 1.217411
2.Si 2.048893 -1.182929 1.219683	2.Si 2.029669 -1.171830 1.217411
3.Si 0.000000 2.365858 1.219683	3.Si 0.000000 2.343660 1.217411
4.Si 0.000000 -2.365858 1.219683	4.Si 0.000000 -2.343660 1.217411
5.Si -2.048893 1.182929 1.219683	5.Si -2.029669 1.171830 1.217411
6.Si -2.048893 -1.182929 1.219683	6.Si -2.029669 -1.171830 1.217411
7.Si 2.048893 1.182929 -1.219683	7.Si 2.029669 1.171830 -1.217411
8.Si 2.048893 -1.182929 -1.219683	8.Si 2.029669 -1.171830 -1.217411
9.Si 0.000000 2.365858 -1.219683	9.Si 0.000000 2.343660 -1.217411
10.Si 0.000000 -2.365858 -1.219683	10.Si 0.000000 -2.343660 -1.217411
11.Si -2.048893 1.182929 -1.219683	11.Si -2.029669 1.171830 -1.217411
12.Si -2.048893 -1.182929 -1.219683	12.Si -2.029669 -1.171830 -1.217411
13.Cr 0.000000 0.000000 0.000000	13.Cr 0.000000 0.000000 0.000000
$^3E_{2g}$, BLYP functional, E=-54.91279167 eV	**$^3E_{2g}$, B3LYP functional, E=-70.02999189 eV**
1.Si 2.056629 1.187395 1.217065	1.Si 2.043987 1.180097 1.211505
2.Si 2.056629 -1.187395 1.217065	2.Si 2.043987 -1.180097 1.211505
3.Si 0.000000 2.374790 1.217065	3.Si 0.000000 2.360193 1.211505
4.Si 0.000000 -2.374790 1.217065	4.Si 0.000000 -2.360193 1.211505
5.Si -2.056629 1.187395 1.217065	5.Si -2.043987 1.180097 1.211505
6.Si -2.056629 -1.187395 1.217065	6.Si -2.043987 -1.180097 1.211505
7.Si 2.056629 1.187395 -1.217065	7.Si 2.043987 1.180097 -1.211505
8.Si 2.056629 -1.187395 -1.217065	8.Si 2.043987 -1.180097 -1.211505
9.Si 0.000000 2.374790 -1.217065	9.Si 0.000000 2.360193 -1.211505
10.Si 0.000000 -2.374790 -1.217065	10.Si 0.000000 -2.360193 -1.211505
11.Si -2.056629 1.187395 -1.217065	11.Si -2.043987 1.180097 -1.211505
12.Si -2.056629 -1.187395 -1.217065	12.Si -2.043987 -1.180097 -1.211505
13.Cr 0.000000 0.000000 0.000000	13.Cr 0.000000 0.000000 0.000000
^3A_g, BLYP functional, E=-55.00738839 eV	**^3A_g, B3LYP functional, E=-70.42093292 eV**
1.Si -1.269391 -2.447860 0.000000	1.Si -1.290281 -2.476968 0.000000
2.Si -1.201071 -1.186005 -1.993903	2.Si -1.144890 -1.175599 -1.970498
3.Si -1.201071 -1.186005 1.993903	3.Si -1.144890 -1.175599 1.970498
4.Si -1.206490 1.220840 -2.043973	4.Si -1.251151 1.199363 -2.090099
5.Si -1.206490 1.220840 2.043973	5.Si -1.251151 1.199363 2.090099
6.Si -1.225763 2.401961 0.000000	6.Si -1.123497 2.340300 0.000000
7.Si 1.225763 -2.401961 0.000000	7.Si 1.123497 -2.340300 0.000000
8.Si 1.206490 -1.220840 -2.043973	8.Si 1.251151 -1.199363 -2.090099
9.Si 1.206490 -1.220840 2.043973	9.Si 1.251151 -1.199363 2.090099
10.Si 1.201071 1.186005 -1.993903	10.Si 1.144890 1.175599 -1.970498
11.Si 1.201071 1.186005 1.993903	11.Si 1.144890 1.175599 1.970498

12.Si 1.269391 2.447860 0.000000 13.Cr 0.000000 0.000000 0.000000	12.Si 1.290281 2.476968 0.000000 13.Cr 0.000000 0.000000 0.000000
^3B_g, BLYP functional, E=-55.02321256 eV 1.Si -1.189603 -2.303948 0.000000 2.Si -1.279884 -1.230252 -2.127537 3.Si -1.279884 -1.230252 2.127537 4.Si -1.163943 1.122462 -2.078055 5.Si -1.163943 1.122462 2.078055 6.Si -1.200773 2.335886 0.000000 7.Si 1.200773 -2.335886 0.000000 8.Si 1.163943 -1.122462 -2.078055 9.Si 1.163943 -1.122462 2.078055 10.Si 1.279884 1.230252 -2.127537 11.Si 1.279884 1.230252 2.127537 12.Si 1.189603 2.303948 0.000000 13.Cr 0.000000 0.000000 0.000000	**^3B_g, B3LYP functional, E=-70.43418178 eV** 1.Si -1.160487 -2.268261 0.000000 2.Si -1.288710 -1.243003 -2.136099 3.Si -1.288710 -1.243003 2.136099 4.Si -1.122237 1.114724 -2.040524 5.Si -1.122237 1.114724 2.040524 6.Si -1.226878 2.367051 0.000000 7.Si 1.226878 -2.367051 0.000000 8.Si 1.122237 -1.114724 -2.040524 9.Si 1.122237 -1.114724 2.040524 10.Si 1.288710 1.243003 -2.136099 11.Si 1.288710 1.243003 2.136099 12.Si 1.160487 2.268261 0.000000 13.Cr 0.000000 0.000000 0.000000
$^3A'$, BLYP functional, E=-55.01950399 eV 1.Si 0.041246 -1.231914 -2.404295 2.Si -1.993006 -1.360143 -1.193041 3.Si 2.068450 -1.046599 -1.217186 4.Si -1.993006 -1.360143 1.193041 5.Si 2.068450 -1.046599 1.217186 6.Si 0.041246 -1.231914 2.404295 7.Si -0.038622 1.237645 -2.447314 8.Si -2.042408 1.042897 -1.227725 9.Si 1.967848 1.357947 -1.189448 10.Si -2.042408 1.042897 1.227725 11.Si 1.967848 1.357947 1.189448 12.Si -0.038622 1.237645 2.447314 13.Cr -0.002480 0.000543 0.000000	