Supporting Information

Redox-active Molecular Wires Derived From Dinuclear Ferrocenyl/Ruthenium(II) Alkynyl Complexes: Covalent Attachment to Hydrogen-Terminated Silicon Surfaces

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Contents

1. Synthesis of 7 and Desilylation Procedure to give 3 and 4

Ethynylferrocene[1] and *cis*-[Ru(κ^2-dppe)$_2$Cl$_2$][2] (dppe = 1,2-bis(diphenylphosphino)ethane), were obtained following published procedures.

*trans-[(κ^2-dppe)$_2$ClRu{=C=CH(η^5-C$_5$H$_4$)Fe(η^5-C$_5$H$_5$)}][PF$_6$] (**7**).* In a Schlenk flask, *cis*-[RuCl$_2$(κ^2-dppe)$_2$] (0.484 g, 0.50 mmol) and NaPF$_6$ (0.092 g, 0.55 mmol) were stirred in CH_2Cl_2 (20 mL) for 12 h under nitrogen with the exclusion of light. Ethynylferrocene (0.116 g, 0.55 mmol) was added to the resulting deep red solution, and the reaction mixture was heated at 40 °C for 48 h. After cooling to room temperature, the inorganic salts were removed by vacuum filtration with a sintered glass funnel and were rinsed with CH_2Cl_2 (3 × 5 mL). The combined filtrates were concentrated under reduced pressure to ≈ 5 mL. Et_2O was added to the CH_2Cl_2 extract to precipitate the vinylidene salt, which was collected by suction filtration on a sintered glass funnel, washed with Et_2O (3 × 5 mL), hexanes (3 × 5 mL) and finally dried in *vacuo*, affording the title compound as a brown solid (0.615 g; 95 %).

Calcd. for $C_{64}H_{58}ClF_6FeP_5Ru$: C: 59.66 %, H: 4.54 %; found: C: 59.70 %, H: 4.72 %. HRMS (ESI): calcd.: 1317.1687 $[M\text{-}PF_6\text{-}Cl+CH_3CN+Na]^+$, found: 1317.1799. IR (KBr, cm^{-1}): 1648 (m, Ru=C=C), 839 (s, P-F). $^{31}P\{^1H\}$ NMR (121 MHz, $CDCl_3$): δ 43.8 (s, PPh_2), -143.1 (sept, $^1J_{P,F}$ = 712 Hz, PF_6). ^1H NMR (300 MHz, $CDCl_3$): δ 7.75 – 6.74 (m, 40H, $H_{aromatics}$), 4.32 (m, 1H, C_5H_5), 4.20 – 3.95 (m, 6H, C_5H_4 or C_5H_5), 3.56 (s, 2H, C_5H_4 or C_5H_5), 3.28 (broad s, 1H, =C=C*H*), 2.98 and 2.69 (2 × m, 2 × 4H, $CH_{2/dppe}$).

[1] Doisneau, G.; Balavoine, G.; Fillebeen-Khan, T. *J. Organomet. Chem.* **1992**, *425*, 113-117.
[2] Green, K. A.; Cifuentes, M. P.; Corkery, T. C.; Samoc, M.; Humphrey, M. G. *Angew. Chem., Int. Ed. Engl.* **2009**, *48*, 7867-7870.

*Desilylation of **9** and **11***. In a Schlenk flask, the complex **9** or **11 (**0.163 g, 0.125 mmol) was dissolved in THF (10 mL) under nitrogen. [N^{n}Bu$_4$]F (TBAF) (0.13 mL, 0.13 mmol, 1.0 M in THF) was added dropwise, and the orange solution was stirred for 1 h. The reaction was then quenched with water (0.10 mL), and the solvent was removed *in vacuo* to give an orange solid. This solid was purified by column chromatography (basic alumina, 3 × 10 cm). An orange band was collected following elution with CH_2Cl_2 (containing 1% Et_3N), and then concentrated under reduced pressure to ≈ 5 mL. A precipitate was formed by addition of MeOH, collected by filtration, washed with MeOH (3 × 5 mL) and hexanes (3 × 5 mL), and finally dried *in vacuo*, affording the desilylated complex **3** or **4** as an air-stable orange solid (0.149 g or 0.148 g, respectively).

Spectroscopic Characterization of the Complexes. Diagnostic signatures of **2-4, 9** and **11** were obtained from NMR studies in solution. Thus, ^{31}P NMR spectroscopy reveals a *trans*-substituted diamagnetic bis-alkynyl Ru(II) center in all these compounds, as confirmed by the observation of singlets at ca. 54 ppm. In the case of **2**, a second singlet corresponding to the equivalent phosphorus atoms coordinated to the iron center is also observed around 101 ppm with the correct relative intensity ratio. In addition, ^{1}H NMR confirms the presence of the 1,1`-substituted ferrocenyl groups for **3, 4, 9** and **11**, with a singlet for the terminal trimethylsilyl group seen at ca. 0.3 ppm for **9** and **11**, and a singlet for the terminal ethynyl proton observed near 3 ppm in the spectra of **2**, **3** and **4**. The presence of the alkyne bonds is also unambiguously established by ^{13}C NMR spectroscopy, with the alkynyl carbon atoms in the alpha position with respect to ruthenium giving rise to characteristic quintets due to their coupling with the four equivalent phosphorus atoms ($^2J_{P,C}$ ~ 15 Hz).[3,4]

[3] Gauthier, N.; Tchouar, N.; Justaud, F.; Argouarch, G.; Cifuentes, M. P.; Toupet, L.; Touchard, D.; Halet, J.-F.; Rigaut, S.; Humphrey, M. G.; Costuas, K.; Paul, F. *Organometallics* **2009**, *28*, 2253-2266.

The solid-state IR spectra of **2**, **3**, **9**, and **11** in KBr reveal strong $\nu_{C\equiv C}$ bands in the range 2044-2060 cm^{-1}, characteristic of such metal alkynyl complexes, and resulting from the overlap of the two different $\nu_{C\equiv CRu}$ modes of these compounds.[5]**Erreur ! Signet non défini.**,[6] This band is usually found at higher wavenumbers for ferrocenyl-alkynyl Ru(II) complexes than for purely arylethynyl examples, reflecting the fact that the backdonation from ruthenium towards the alkynyl moiety is overall less effective when the electron-rich ferrocenyl group is appended to the alkynyl bond.[7] Another, less intense, $\nu_{C\equiv C}$ mode is also apparent for these complexes. For **3** and **5**, it corresponds to the terminal alkyne appended to the phenylethynyl ligand, while for **9** and **11** it stems from the alkyne appended to the ferrocenyl core. As expected for this second band within each series, terminal alkynes are always found at lower energies (ca. 2140-2050 cm^{-1}) than trimethylsilyl-protected ones (ca. 2200-2100 cm^{-1}).[8] For **2**, **3** and **4**, successful deprotection is also evidenced by a diagnostic $\nu_{\equiv C-H}$ mode near 3290 cm^{-1}.

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[4] Fox, M. A.; Harris, J. E.; Heider, S.; Pérez-Gregorio, V.; M. E. Zakrzewska; Farmer, J. D.; Yufit, D. S.; Howard, J. A. K.; Low, P. J. *J. Organomet. Chem.* **2009**, *694*, 2350-2358.

[5] Gauthier, N.; Olivier, C.; Rigaut, S.; Touchard, D.; Roisnel, T.; Humphrey, M. G.; Paul, F. *Organometallics* **2008**, *27*, 1063-1072.

[6] Gauthier, N.; Argouarch, G.; Paul, F.; Toupet, L.; Ladjarafi, A.; Costuas, K.; Halet, J.-F.; Samoc, M.; Cifuentes, M. P.; Corkery, T. C.; Humphrey, M. G. *Chem. Eur. J.* **2011**, *17*, 5561-5577.

[7] Paul, F.; Mevellec, J.-Y.; Lapinte, C. *J. Chem. Soc., Dalton Trans.* **2002**, 1783-1790.

[8] Bellamy, L. J. *The infrared spectra of complex molecules*; Methuen & co Ldt: London, 1955.

2. Additional Structural Data for Complex 11

Table S1. Crystal Data, Data Collection, and Refinement Parameters for **11**.

formula	$C_{77}H_{70}Fe_1P_4Ru_1Si_1$
fw	1304.22
cryst. syst.	triclinic
space group	*P*-1
a (Å)	9.5320(10)
b (Å)	13.7554(15)
c (Å)	27.635(3)
α (deg)	81.394(5)
β (deg)	83.466(4)
γ (deg)	71.709(4)
V (Å^3)	3393.0(6)
Z	2
$D_{(calcd)}$ (g cm^{-3})	1.277
crystal size (mm^3)	$0.56 \times 0.14 \times 0.09$
F(000)	1352
abs. coef̃ (mm^{-1})	0.590
N° total refl. / N° unique refl.	41503 / 15295 [$R_{(int)}$ = 0.0384]
N° variables / N° refl. > 2σ(I)	757 / 11850
final R	0.0680
wR	0.1605
Goodness of fit / F^2 (S)	1.029

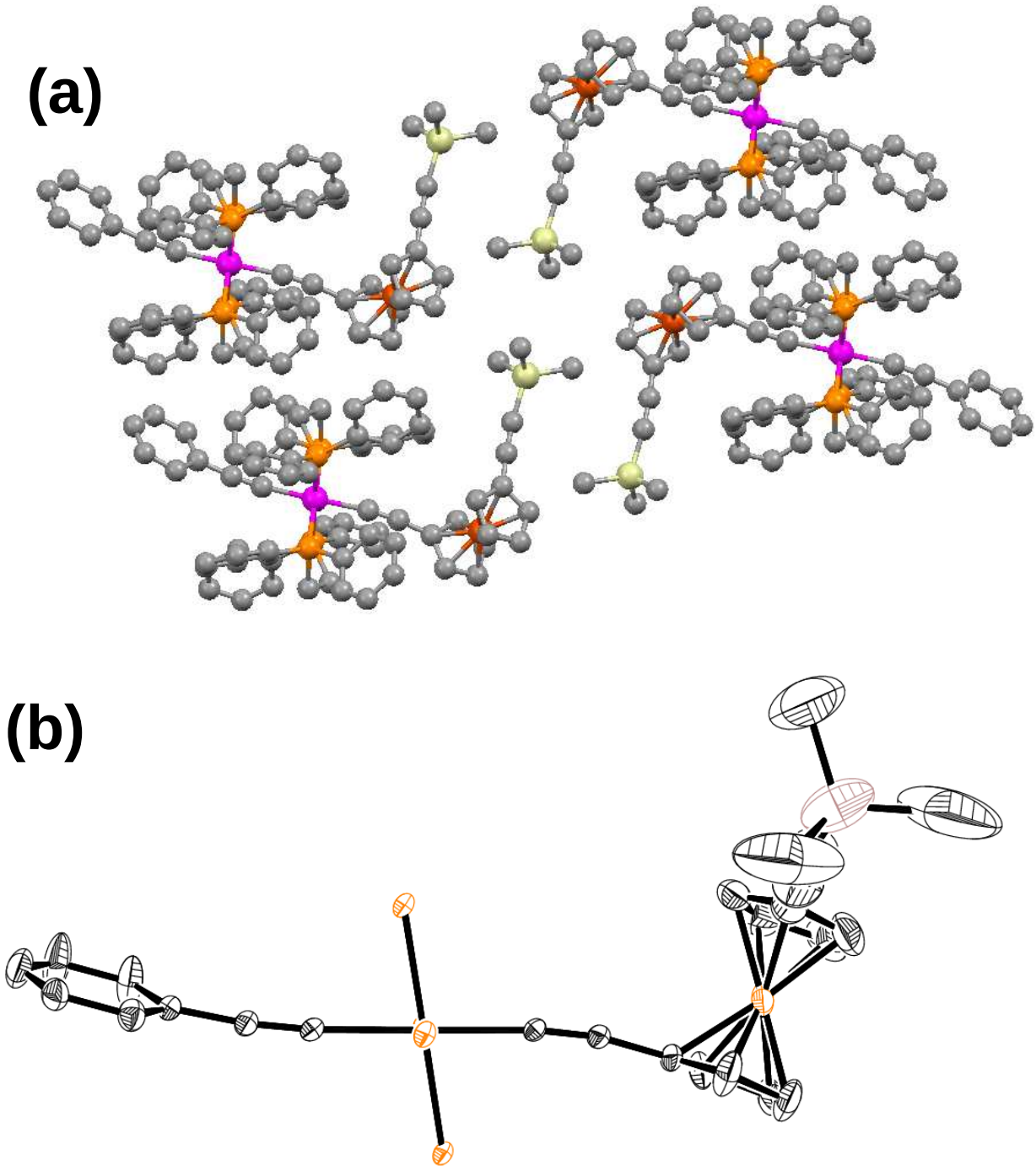

Figure S1. (a) Crystal packing of **11**. (b) View of selected atoms of **11** revealing the S-shaped conformation of the metal-alkynyl axis.

3. Cyclic Voltammograms of Complexes 3, 4 and 11 in CH_2Cl_2

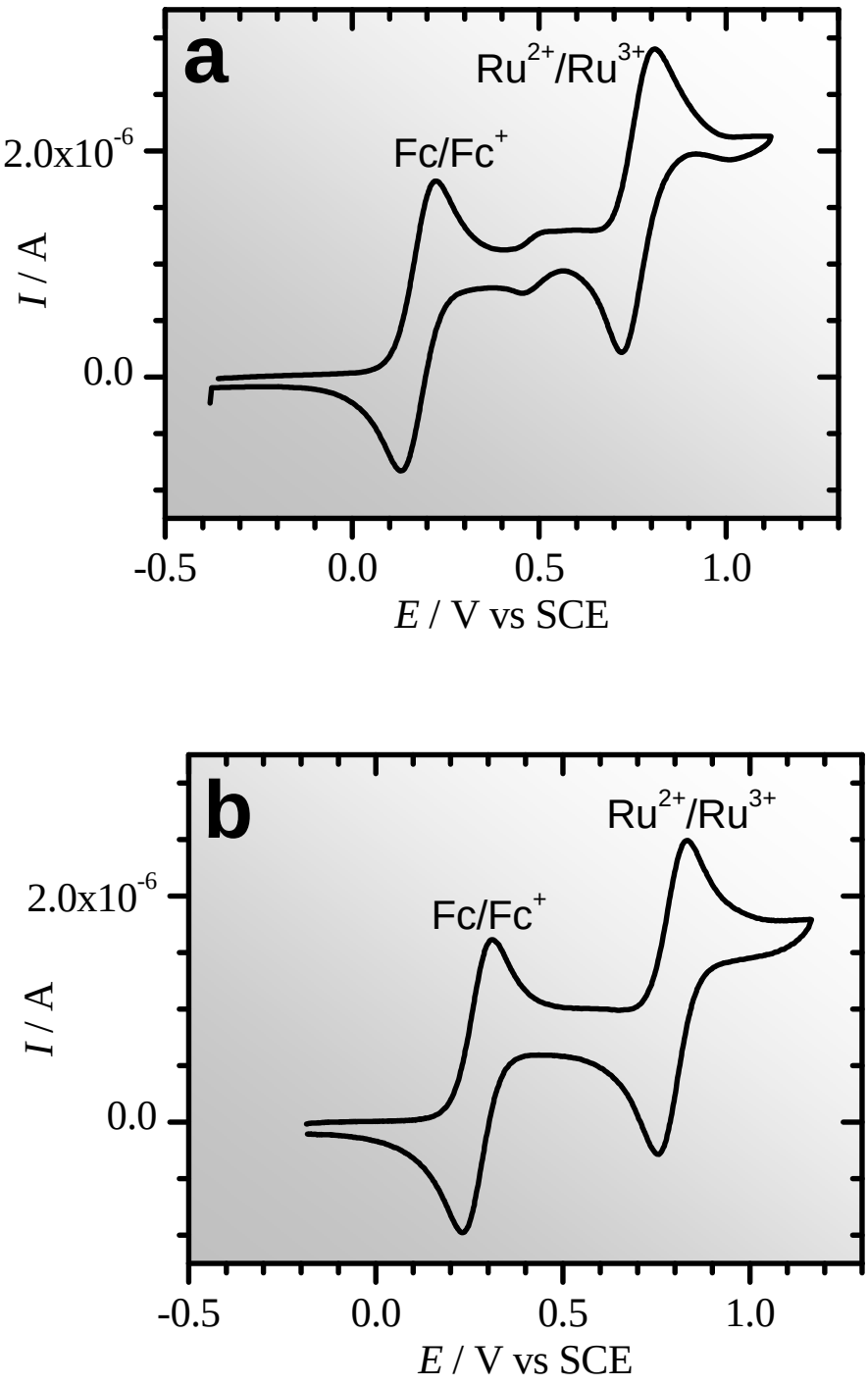

Figure S2. Cyclic voltammograms (CVs) at a scan rate of 0.1 V s^{-1} of **3** (a) and **4** (b) at ca. 1 mM complex in CH_2Cl_2 + 0.1 M [*n*-Bu_4N][PF_6] on a platinum (1 mm diameter) disk electrode. Traces of ferrocene, used for the calibration, are visible at ca. 0.46 V in CV (a).

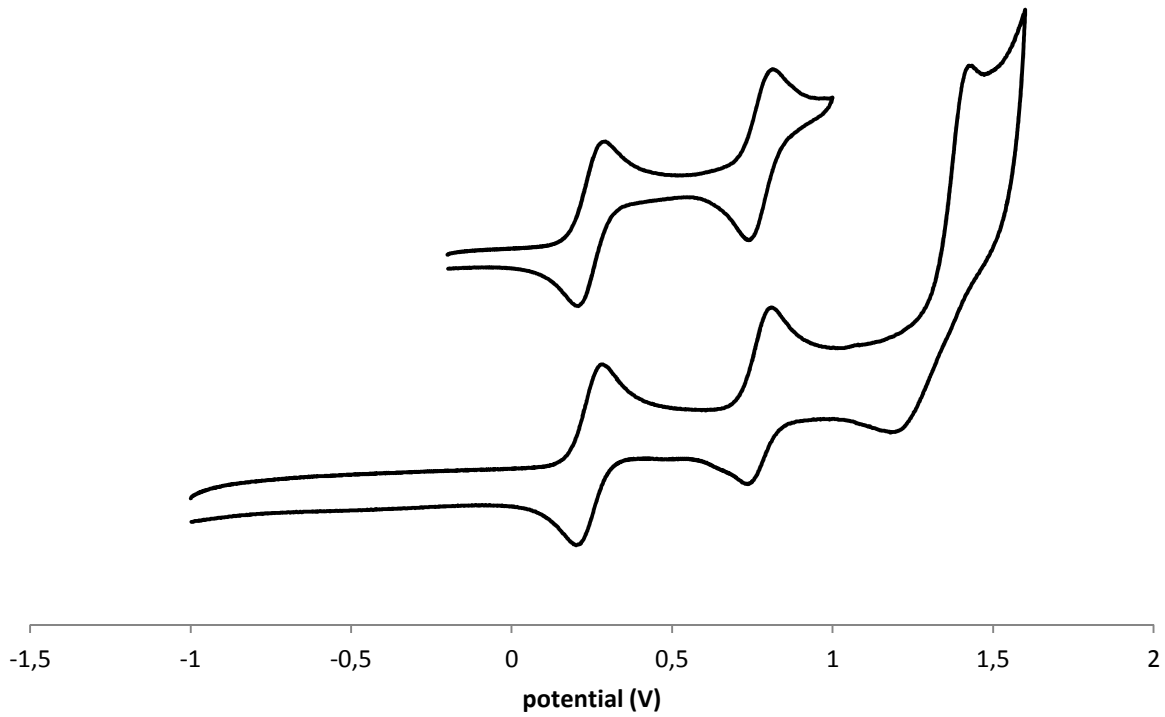

Figure S3. Cyclic voltammograms at a scan rate of 0.1 V s^{-1} on a platinum (1 mm diameter) disk electrode of **11** at ca. 1 mM complex in CH_2Cl_2 + 0.1 M [*n*-Bu_4N][PF_6] within the potential ranges -1.0 – 1.6 V (bottom trace) and -0.2 -1.0 V (top trace). In both cases, the ferrocene/ferrocenium couple was found at 0.45 V vs SCE reference electrode.

4. XPS Data for Si-2

Table S2. XPS data collected for **Si-2**.

Peak	Binding energy / eV	Assignment
C 1s	285.0	C-C, C=C, C≡C
	287.1	C-P
	283.0	C-Si
Fe $2p_{3/2}$	707.9, 709.9	Fe(II)
	712.1	Fe(III)
Ru $3d_{5/2}$	280.6	Ru(II)
Si 2p	99.2	Si-Si
	103.1	SiO_x

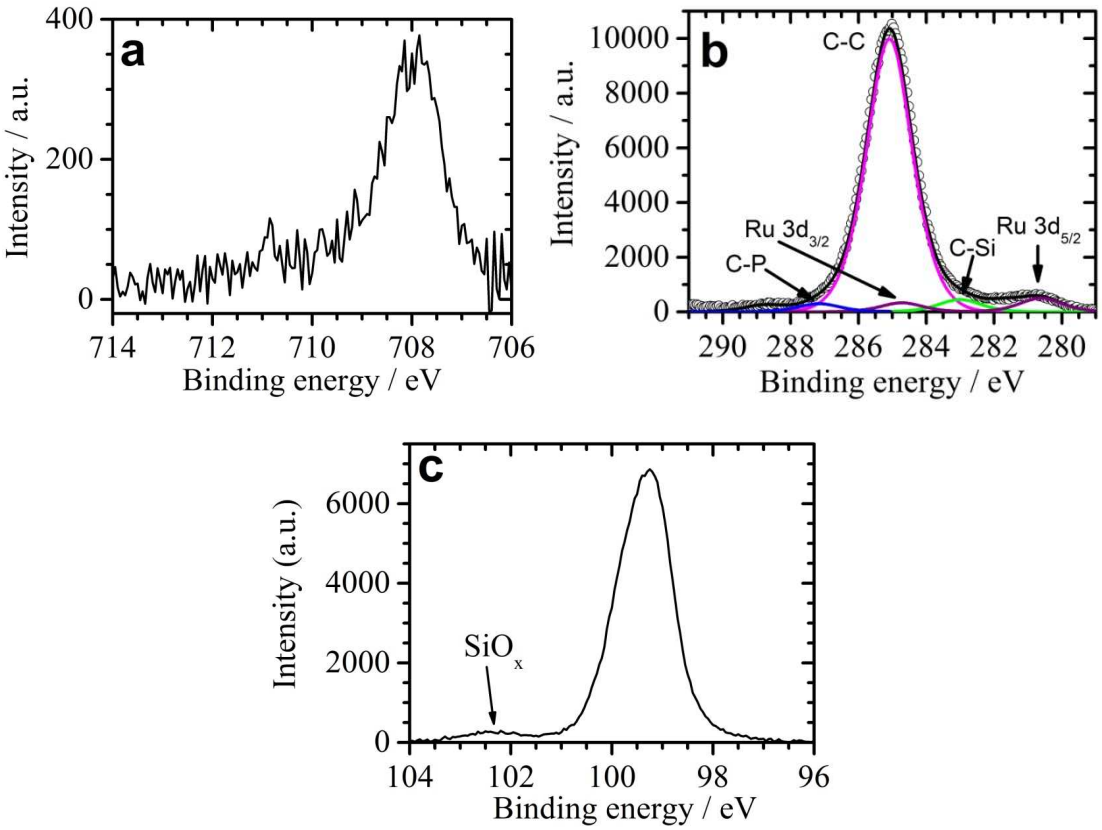

Figure S4. High-resolution XP Fe $2p_{3/2}$ (a), C 1s and Ru 3d (b) and Si 2p (c) spectra of **Si-2** surfaces recorded at normal incidence. For (b), the black circles are experimental data and the black lines are the fitted curves that were generated using combinations of Gaussian-Lorentzian functions, each corresponding to a different contribution. For (c), the silicon oxides region is highlighted.

5. Electrochemical Data for Si-2 in CH_3CN

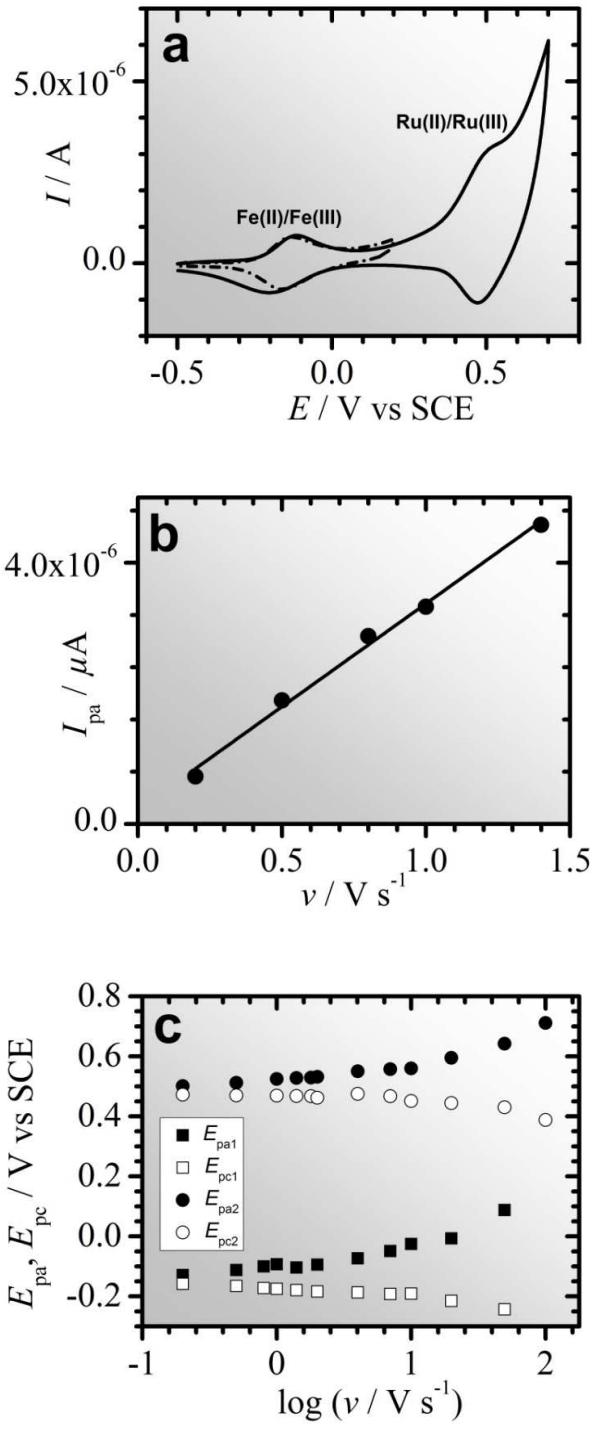

Figure S5. (a) Cyclic voltammograms in CH_3CN + 0.1 M [*n*-Bu_4N][ClO_4] of **Si-2** at 0.2 V s^{-1} scan rate; first (dashed trace) and second (solid trace) scans. (b) Corresponding I_{pa} - *v* plot for the first Fe-based redox system. (c) E_{pa}, E_{pc} – log *v* plots for the two attached metallic centers.

6. Computational Details

DFT calculations (spin unrestricted for all open shell systems) were performed on gas phase molecules using the Gaussian 03, Revision D.02, program package, the B3LYP functional and the LanL2DZ basis set. The latter employs the Dunning/Huzinaga valence double zeta D95V [1] basis set for first row atoms and the Los Alamos Effective Core Potential plus DZ on atoms from Na-Bi.[2–4]

1 T. H. Dunning Jr and P. J. Hay, Modern Theoretical Chemistry, Plenum, New York, 1976.

2 P. J. Hay and W. R. Wadt, J. Chem. Phys., 1985, 82, 270.

3 W. R. Wadt and P. J. Hay, J. Chem. Phys., 1985, 82, 284.

4 P. J. Hay and W. R. Wadt, J. Chem. Phys., 1985, 82, 299.

Full parameters for common basis sets are available at https://bse.pnl.gov/bse/portal

Parameters for the LanL2DZ basis set are reproduced next.

7. The LanL2DZ Basis Set

When publishing results obtained from use of the Basis Set Exchange (BSE) software and the EMSL Basis Set Library, please cite:

The Role of Databases in Support of Computational Chemistry Calculations
Feller, D., J. Comp. Chem., 17(13), 1571-1586, 1996.

Basis Set Exchange: A Community Database for Computational Sciences
Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L.
J. Chem. Inf. Model., 47(3), 1045-1052, 2007, doi:10.1021/ci600510j.

```
!  LANL2DZ ECP  EMSL  Basis Set Exchange Library   4/26/11 8:55 AM
! Elements                             References
! --------                             ----------
! H  - Ne: T. H. Dunning Jr. and P. J. Hay, in Methods of Electronic Structure
! Theory, Vol. 2, H. F. Schaefer III, ed., PLENUM PRESS (1977)
! Na - Hg: P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 270 (1985).
! P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 284 (1985).
! P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 299 (1985).
!


****
H     0
S   3   1.00
     19.2384000              0.0328280
      2.8987000              0.2312040
      0.6535000              0.8172260
S   1   1.00
      0.1776000              1.0000000
****
C     0
S   7   1.00
   4233.0000000              0.0012200
    634.9000000              0.0093420
    146.1000000              0.0454520
     42.5000000              0.1546570
     14.1900000              0.3588660
      5.1480000              0.4386320
      1.9670000              0.1459180
S   2   1.00
      5.1480000             -0.1683670
      0.4962000              1.0600910
S   1   1.00
      0.1533000              1.0000000
P   4   1.00
     18.1600000              0.0185390
      3.9860000              0.1154360
      1.1430000              0.3861880
      0.3594000              0.6401140
P   1   1.00
      0.1146000              1.0000000
****
P     0
S   2   1.00
      1.5160000             -0.5862089
      0.3369000              1.2994376
S   1   1.00
      0.1211000              1.0000000
P   2   1.00
      3.7050000             -0.0691472
      0.3934000              1.0161988
P   1   1.00
      0.1190000              1.0000000
****
S     0
S   2   1.00
      1.8500000             -0.5324335
      0.4035000              1.2763801
S   1   1.00
      0.1438000              1.0000000
```

```
P   2   1.00
      4.9450000             -0.0608116
      0.4870000              1.0132686
P   1   1.00
      0.1379000              1.0000000
****
Ru     0
S   3   1.00
      2.5650000             -1.0431056
      1.5080000              1.3314786
      0.5129000              0.5613065
S   4   1.00
      2.5650000              0.8770128
      1.5080000             -1.2634660
      0.5129000             -0.8384987
      0.1362000              1.0637773
S   1   1.00
      0.0417000              1.0000000
P   3   1.00
      4.8590000             -0.0945755
      1.2190000              0.7434798
      0.4413000              0.3668144
P   2   1.00
      0.5725000             -0.0880864
      0.0830000              1.0283970
P   1   1.00
      0.0250000              1.0000000
D   3   1.00
      4.1950000              0.0485729
      1.3770000              0.5105223
      0.4828000              0.5730028
D   1   1.00
      0.1501000              1.0000000
****

! Elements                               References
! --------                               ----------
! Na - Hg: P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 270 (1985).
!          P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 284 (1985).
!          P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 299 (1985).
!


P     0
P-ECP     2     10
d   potential
  5
1    462.1211423            -10.0000000
2     93.6863701            -79.4864658
2     21.2349094            -28.3668251
2      6.3388415             -9.8577589
2      2.0620684             -1.0163783
s-d potential
  5
0     78.0831823              3.0000000
1     58.9576810             12.9104154
2     36.0571255            150.0250298
2     11.2464453             71.7083146
2      2.6757561             23.0397012
p-d potential
  6
0     75.1617880              5.0000000
1     57.4544041              6.3446507
2     47.9481748            198.5585104
2     18.4588360            111.1470820
2      5.9414190             40.3944144
2      1.8487507              6.4483233
S     0
S-ECP     2     10
d   potential
  5
1    532.6685222            -10.0000000
2    108.1342248            -85.3593846
2     24.5697664            -30.4513290
2      7.3702438            -10.3745886
2      2.3712569             -0.9899295
s-d potential
  5
0    106.3176781              3.0000000
1    100.8245833             10.6284036
2     53.5858472            223.6360469
2     15.3706332             93.6460845
2      3.1778402             28.7609065
p-d potential
  6
0    101.9709185              5.0000000
1     93.2808973              6.0969842
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2     65.1431772            285.4425500
2     24.6347440            147.1448413
2      7.8120535             53.6569778
2      2.3112730              8.9249559
RU     0
RU-ECP     3     28
f potential
  5
0    554.3796303             -0.0515270
1    155.1066871            -20.1816536
2     48.4976263           -105.9966915
2     14.7701594            -42.2166788
2      5.2077363             -3.7675024
s-f potential
  5
0     66.7118060              2.9578344
1     77.3503632             25.3748707
2     18.3571445            536.1262372
2     11.8404727           -651.2057221
2      8.1179479            381.3816943
p-f potential
  5
0     54.9937915              4.9651557
1     13.9399212             23.8861501
2     15.2118246            464.4631344
2     10.5460691           -714.4451788
2      7.5539486            377.5503594
d-f potential
  4
0     60.3444595              3.0352988
1     45.2100305             23.2901723
2     19.1190074            146.0926620
2      4.2712090             28.9129770
```

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8. Comparison between Experimental (X-ray Structural Study) and Computed (DFT) Bond Lengths for 4

Table S3. Selected Computed Bond Lengths (Å) for [(HC≡C-η^5-C_5H_4)Fe(η^5-C_5H_4C≡C)-*trans*-(κ^2-dppe)$_2$Ru{C≡C(4-C_6H_4C≡CH)}] (**4**) Compared to Available Experimental X-ray Data for [(Me_3SiC≡C-η^5-C_5H_4)Fe(η^5-C_5H_4C≡C)-*trans*-(κ^2-dppe)$_2$Ru{C≡C(4-C_6H_4C≡CH)}] (**11**) [Given in Brackets].

Bonds	**Bond Lengths**
Ru1-P1	2.466 [2.3536(11)]
Ru1-P2	2.483 [2.3565(11)]
Ru1-P3	2.470 [2.3531(11)]
Ru1-P4	2.472 [2.3574(11)]
Ru-C_α	2.0825 [2.070(4)]
C_α-C_β	1.2485 [1.211(6)]
C_β-C_{Cp}	1.4275 [1.439(6)]
Ru-$C_{\alpha'}$	2.0725 [2.066(4)]
$C_{\alpha'}$- $C_{\beta'}$	1.2485 [1.216(6)]
$C_{\beta'}$-C_{Ph}	1.4365 [1.435(6)]
$C_{Cp'}$-$C_{\alpha''}$	1.425 [1.345(11)]
Fe-Cp’	1.729 [1.661]
Fe-Cp’’	1.728 [1.620]
$C_{\alpha''}$-$C_{\beta''}$	1.225 [1.272(12)]

9. Input Files, Cartesian Coordinates of Optimized Geometry, HOMO, SOMO, SOMO-1 and Spin Density

Geometry Optimization of Complex 3

Input file:

```
%chk=FedP3SP

#B3LYP/LanL2DZ opt

FedP3SP

  0  1
```

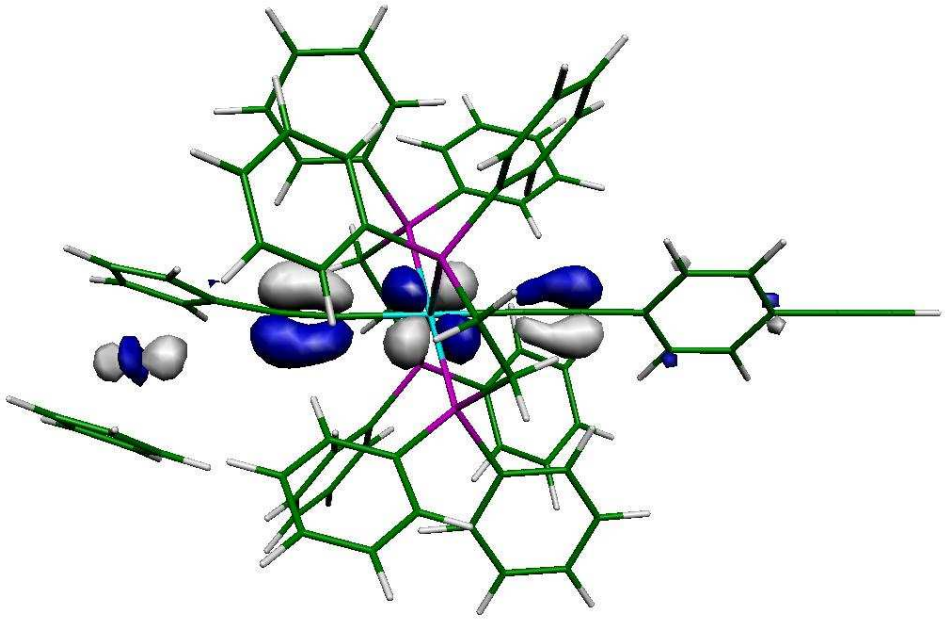
Cartesians Coordinates for the Optimized Geometry of Complex **3** (`-3099.9341721 Hartrees`)

Ru	0.38016	0.10493	0.02105
P	0.42486	-1.48343	-1.86827
P	0.34327	1.77610	-1.81702
C	-0.84657	-2.87744	-2.03400
C	-1.84148	-3.06979	-1.05794
C	-2.78594	-4.10620	-1.19816
C	-2.74919	-4.95432	-2.31914
C	-1.76362	-4.75824	-3.30775
C	-0.81941	-3.72676	-3.16480
C	2.02430	-2.39416	-2.31883
C	2.21431	-3.74114	-1.94470
C	3.40867	-4.41271	-2.26355
C	4.43450	-3.74678	-2.95957
C	4.26240	-2.39522	-3.31360
C	3.07160	-1.72230	-2.98575
C	0.08808	-0.48562	-3.48492
C	-0.58380	3.41444	-1.67328
C	-1.98539	3.47828	-1.82079
C	-2.65595	4.71196	-1.72224
C	-1.93802	5.89422	-1.46446
C	-0.54038	5.83431	-1.29806
C	0.13095	4.60272	-1.39933
C	1.87108	2.34301	-2.79796
C	3.17199	1.94300	-2.43462
C	4.28430	2.35515	-3.19780
C	4.10672	3.16467	-4.33357
C	2.80645	3.56505	-4.70503
C	1.69884	3.15922	-3.94150
C	-0.59629	0.86026	-3.20172
P	0.44412	-1.55124	1.85356
P	0.33052	1.70456	1.90290
C	-1.06790	-2.12775	2.84863
C	-2.36776	-1.69112	2.52574
C	-3.46493	-2.08387	3.32107
C	-3.27479	-2.91104	4.44138

C	-1.97591	-3.35217	4.76715
C	-0.88193	-2.96294	3.97604
C	1.39761	-3.17272	1.70407
C	0.70386	-4.37274	1.42872
C	1.39703	-5.59209	1.32490
C	2.79557	-5.62718	1.48941
C	3.49328	-4.43259	1.74661
C	2.80098	-3.21128	1.84783
C	1.37870	-0.62198	3.23418
C	1.60678	3.09629	2.06312
C	2.60481	3.27948	1.08847
C	3.56450	4.30136	1.23125
C	3.53810	5.14726	2.35475
C	2.54480	4.96550	3.33848
C	1.58692	3.94678	3.19293
C	-1.26622	2.62094	2.34918
C	-1.46045	3.95752	1.94159
C	-2.65191	4.63687	2.25316
C	-3.67065	3.98982	2.97647
C	-3.49320	2.64939	3.36757
C	-2.30555	1.96766	3.04579
C	0.67434	0.71279	3.52071
C	2.43501	-0.01693	0.21866
C	3.66456	-0.11392	0.41290
C	5.07594	-0.23006	0.62598
C	5.82218	-1.30736	0.06593
C	7.20205	-1.41862	0.27236
C	7.90259	-0.45930	1.04933
C	7.16695	0.61511	1.61407
C	5.78724	0.72647	1.40735
C	-1.68663	0.24192	-0.19382
C	-2.89865	0.40292	-0.44096
C	-4.23034	0.74355	-0.82792
C	-5.20592	1.48933	-0.05401
C	-6.37075	1.71656	-0.87230
C	-6.14678	1.08605	-2.15219
C	-4.84422	0.46785	-2.11746
Fe	-6.09712	-0.35311	-0.62693
C	-5.76744	-2.20017	0.35929
C	-6.28856	-2.43602	-0.96509
C	-7.58321	-1.80491	-1.05469
C	-7.86254	-1.17713	0.21474
C	-6.74011	-1.42123	1.08814
C	9.31833	-0.57240	1.25793
C	10.52753	-0.66859	1.43454
H	-1.89655	-2.39705	-0.21055
H	-3.54612	-4.24840	-0.43409
H	-3.47821	-5.75465	-2.42475
H	-1.72710	-5.40628	-4.18038
H	-0.05297	-3.60029	-3.92609
H	1.43705	-4.27603	-1.40893
H	3.53281	-5.45068	-1.96455
H	5.35407	-4.26823	-3.21533
H	5.05300	-1.86026	-3.83442
H	2.98302	-0.67252	-3.24666
H	1.04472	-0.32903	-3.99246
H	-0.53821	-1.10690	-4.13347

H	-2.56390	2.57960	-1.99739
H	-3.73652	4.73932	-1.83825
H	-2.45790	6.84719	-1.39484
H	0.02753	6.73945	-1.09560
H	1.21030	4.57800	-1.27991
H	3.31900	1.30760	-1.56776
H	5.28109	2.03934	-2.89890
H	4.96505	3.48216	-4.92142
H	2.65710	4.19326	-5.58019
H	0.70546	3.49514	-4.22932
H	-1.61735	0.70793	-2.84582
H	-0.61650	1.48363	-4.10292
H	-2.52371	-1.04599	1.66559
H	-4.46188	-1.73635	3.06387
H	-4.12351	-3.21214	5.05124
H	-1.81687	-3.99574	5.62925
H	0.11178	-3.32317	4.23114
H	-0.37607	-4.36631	1.30964
H	0.84544	-6.50714	1.12193
H	3.33217	-6.57069	1.41860
H	4.57409	-4.44259	1.86420
H	3.36206	-2.30022	2.02232
H	1.41220	-1.24618	4.13445
H	2.39649	-0.45238	2.87555
H	2.65155	2.61288	0.23686
H	4.32975	4.42663	0.46874
H	4.27981	5.93505	2.46572
H	2.51457	5.61362	4.21131
H	0.81729	3.82996	3.95259
H	-0.68881	4.47796	1.38371
H	-2.78003	5.66560	1.92560
H	-4.58848	4.51776	3.22538
H	-4.27553	2.13094	3.91766
H	-2.21295	0.92641	3.33758
H	1.29034	1.34087	4.17241
H	-0.28105	0.54060	4.02548
H	5.29858	-2.04571	-0.53426
H	7.75328	-2.24726	-0.16536
H	7.69028	1.35608	2.21323
H	5.23703	1.55488	1.84598
H	-5.04472	1.84811	0.95210
H	-7.25746	2.26070	-0.57759
H	-6.83395	1.07445	-2.98691
H	-4.37897	-0.09588	-2.91418
H	-4.81043	-2.53215	0.73323
H	-5.78680	-2.97495	-1.75646
H	-8.22543	-1.79207	-1.92457
H	-8.75149	-0.61430	0.46419
H	-6.64863	-1.07355	2.10806
H	11.57870	-0.75167	1.58892

Figure S6. HOMO of complex **3** (-4.42 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.



Geometry Optimization of Complex 3^+

Input file:

```
%chk=FedP3SP21SP

#B3LYP/LanL2DZ opt

%chk=FedP3SP21SP

  1  2
```

Cartesians Coordinates for the Optimized Geometry of Complex **3^+** (-3099.7441628 Hartrees)

Ru	0.35252	0.10394	0.00103
P	0.41846	-1.48954	-1.91890
P	0.41689	1.79963	-1.87291
C	-0.89419	-2.83851	-2.08548
C	-1.84563	-3.06584	-1.07410
C	-2.80375	-4.08928	-1.21555
C	-2.82459	-4.88765	-2.37301
C	-1.88148	-4.65709	-3.39482
C	-0.92105	-3.64128	-3.25006

C	2.00073	-2.43650	-2.33115
C	2.13199	-3.79666	-1.98121
C	3.30680	-4.50390	-2.29487
C	4.36638	-3.86140	-2.96152
C	4.24971	-2.49803	-3.29287
C	3.07976	-1.78747	-2.96965
C	0.14464	-0.46874	-3.52717
C	-0.48459	3.44673	-1.72703
C	-1.87728	3.54181	-1.93080
C	-2.52512	4.78805	-1.84206
C	-1.79239	5.95026	-1.53883
C	-0.40377	5.85860	-1.32063
C	0.24591	4.61496	-1.41266
C	1.97958	2.32265	-2.80858
C	3.26472	1.89390	-2.42441
C	4.39695	2.28916	-3.16600
C	4.25366	3.10901	-4.29905
C	2.96853	3.53761	-4.69006
C	1.83983	3.15000	-3.94882
C	-0.52131	0.88779	-3.25656
P	0.41928	-1.58021	1.86206
P	0.31872	1.70083	1.92323
C	-1.11357	-2.12707	2.83202
C	-2.39164	-1.60786	2.55010
C	-3.49603	-1.97212	3.34771
C	-3.33427	-2.85623	4.42843
C	-2.05727	-3.38141	4.71151
C	-0.95450	-3.01822	3.92016
C	1.35782	-3.20092	1.68794
C	0.65456	-4.38797	1.38257
C	1.33665	-5.61309	1.27881
C	2.73084	-5.66539	1.47203
C	3.43697	-4.48320	1.76091
C	2.75673	-3.25560	1.86417
C	1.35282	-0.64727	3.23513
C	1.60346	3.07940	2.07260
C	2.61398	3.25223	1.10887
C	3.57696	4.26944	1.26107
C	3.53944	5.11969	2.38089
C	2.53158	4.94875	3.35148
C	1.56988	3.93511	3.19853
C	-1.27922	2.62154	2.34331
C	-1.47844	3.93047	1.85418
C	-2.65965	4.63332	2.15083
C	-3.66150	4.03869	2.94048
C	-3.47786	2.72651	3.41544
C	-2.30017	2.01894	3.10963
C	0.65315	0.68875	3.52440
C	2.38828	-0.04522	0.21687
C	3.61187	-0.16680	0.43183
C	5.01880	-0.28038	0.67727
C	5.79966	-1.28133	0.03386
C	7.17305	-1.38950	0.27913
C	7.82364	-0.49905	1.17296
C	7.05004	0.50181	1.81703
C	5.67586	0.60685	1.57636
C	-1.63814	0.26722	-0.21583

C	-2.85851	0.47252	-0.45553
C	-4.16845	0.83175	-0.81412
C	-5.15352	1.52470	0.01304
C	-6.32303	1.76883	-0.78054
C	-6.12071	1.17292	-2.08141
C	-4.82459	0.55727	-2.09304
Fe	-6.03463	-0.32638	-0.58672
C	-5.81120	-2.23519	0.39049
C	-6.28500	-2.42336	-0.95580
C	-7.55990	-1.75434	-1.07489
C	-7.86431	-1.14573	0.19239
C	-6.77704	-1.43549	1.09772
C	9.23245	-0.60821	1.42003
C	10.43527	-0.70072	1.63007
H	-1.85090	-2.44345	-0.18677
H	-3.52256	-4.26905	-0.41990
H	-3.56027	-5.68124	-2.47861
H	-1.88692	-5.27019	-4.29234
H	-0.18285	-3.49652	-4.03551
H	1.32474	-4.31525	-1.47488
H	3.38794	-5.55256	-2.02098
H	5.26780	-4.41238	-3.21793
H	5.06368	-1.98621	-3.80019
H	3.03160	-0.73200	-3.21846
H	1.11792	-0.32649	-4.00527
H	-0.47273	-1.07072	-4.20140
H	-2.46720	2.66165	-2.16020
H	-3.59749	4.84579	-2.00979
H	-2.29292	6.91362	-1.48086
H	0.17435	6.74958	-1.08939
H	1.31986	4.56764	-1.25928
H	3.38695	1.25250	-1.55985
H	5.38280	1.95405	-2.85343
H	5.12728	3.41364	-4.86979
H	2.84709	4.17427	-5.56269
H	0.85977	3.50991	-4.25232
H	-1.55298	0.75537	-2.92317
H	-0.51683	1.50752	-4.16007
H	-2.52857	-0.92110	1.72139
H	-4.47496	-1.55380	3.12903
H	-4.18716	-3.13505	5.04207
H	-1.92086	-4.06759	5.54331
H	0.02147	-3.43986	4.14653
H	-0.42301	-4.37045	1.24625
H	0.78017	-6.52031	1.05723
H	3.25745	-6.61405	1.40367
H	4.51349	-4.51004	1.90788
H	3.32513	-2.35734	2.07737
H	1.37739	-1.27338	4.13411
H	2.37436	-0.48422	2.88599
H	2.66953	2.58792	0.25576
H	4.35318	4.38909	0.50925
H	4.28338	5.90356	2.49886
H	2.49327	5.60113	4.22012
H	0.78974	3.82805	3.94869
H	-0.71548	4.41481	1.25366
H	-2.78991	5.64234	1.76878

H	-4.56621	4.58968	3.18554
H	-4.24102	2.25516	4.03048
H	-2.20008	1.00442	3.48210
H	1.27114	1.30892	4.18128
H	-0.30145	0.51695	4.02931
H	5.31244	-1.96631	-0.65353
H	7.75761	-2.15953	-0.21677
H	7.53907	1.18742	2.50341
H	5.09434	1.37866	2.07367
H	-4.97264	1.86755	1.02135
H	-7.20737	2.30061	-0.45885
H	-6.82624	1.18218	-2.90028
H	-4.37075	0.02790	-2.91900
H	-4.88068	-2.60692	0.79446
H	-5.78113	-2.97582	-1.73615
H	-8.17616	-1.71548	-1.96247
H	-8.74886	-0.56955	0.42598
H	-6.71824	-1.12185	2.13067
H	11.48287	-0.78077	1.81383

Figure S7. SOMO of complex $\mathbf{3}^{+}$ (-7.28 eV) shown with a cutoff of 0.05 $[e/Bohr^3]^{1/2}$.

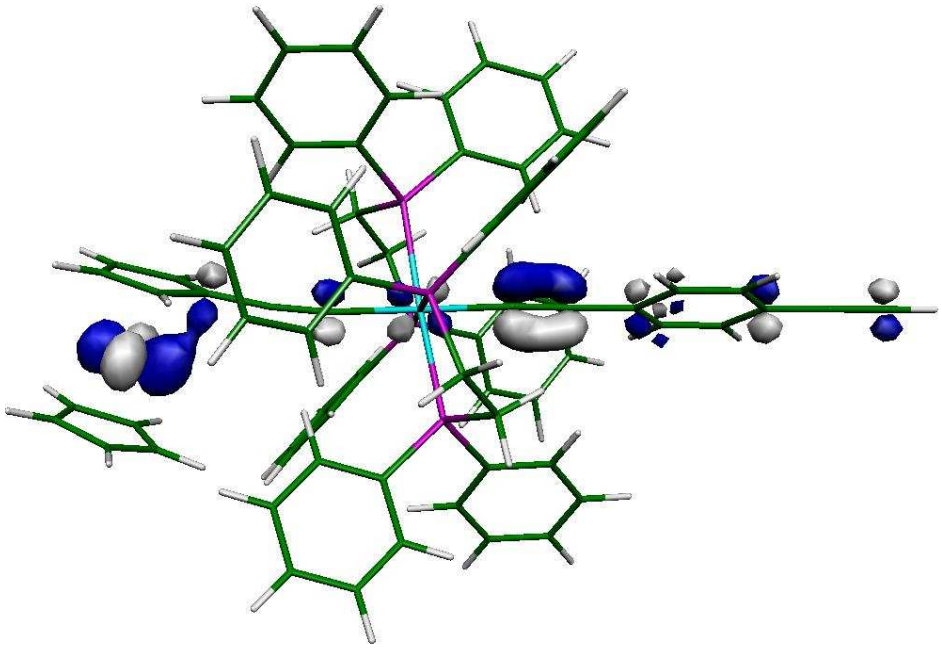
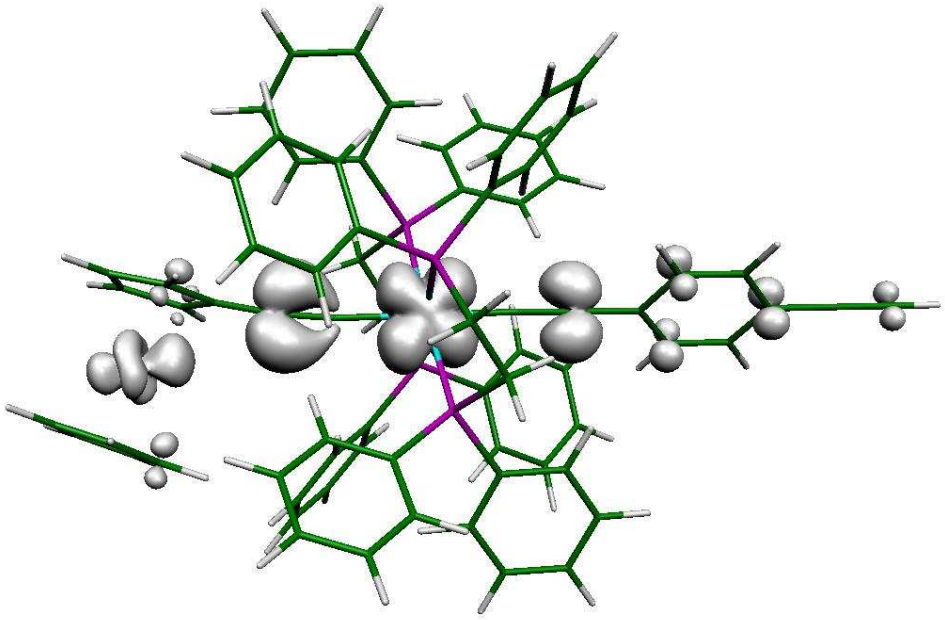


Figure S8. Spin Density for complex $\mathbf{3}^{+}$ shown with a cut-off of 0.002 e/Bohr^3.



Geometry Optimization of Complex $\mathbf{3}^{2+}$

Input file:

```
%chk= FedP3SP22SP

#B3LYP/LanL2DZ opt

%chk= FedP3SP22SP

  2   3
```

Cartesians Coordinates for the Optimized Geometry of Complex $\mathbf{3}^{2+}$ (-3099.4608098Hartrees)

Ru	0.40231	0.11034	-0.00089
P	0.43841	-1.49407	-1.92331
P	0.42445	1.80731	-1.89076
C	-0.88971	-2.82903	-2.05939
C	-1.82445	-3.04261	-1.02960
C	-2.78489	-4.06760	-1.14220
C	-2.82729	-4.87839	-2.29128
C	-1.90316	-4.65839	-3.33277
C	-0.93759	-3.64356	-3.21511
C	2.01149	-2.45274	-2.33688
C	2.14199	-3.80339	-1.95009
C	3.30534	-4.52677	-2.26965
C	4.35330	-3.91039	-2.97862
C	4.23737	-2.55639	-3.34738
C	3.07898	-1.82842	-3.01916

C	0.15596	-0.47473	-3.52827
C	-0.46287	3.46013	-1.75553
C	-1.84540	3.57753	-2.01044
C	-2.47547	4.83433	-1.94703
C	-1.73457	5.98470	-1.61927
C	-0.35594	5.87118	-1.35393
C	0.27622	4.61709	-1.42045
C	1.99419	2.30439	-2.82609
C	3.27651	1.86597	-2.44741
C	4.40895	2.24683	-3.19536
C	4.26684	3.06339	-4.33105
C	2.98399	3.50259	-4.71676
C	1.85511	3.12921	-3.96854
C	-0.51780	0.87807	-3.25898
P	0.37356	-1.59678	1.87630
P	0.37677	1.71456	1.93305
C	-1.17932	-2.10855	2.83078
C	-2.43814	-1.53617	2.56389
C	-3.55288	-1.87545	3.35799
C	-3.42135	-2.78805	4.41969
C	-2.16403	-3.36582	4.68672
C	-1.04988	-3.02687	3.90006
C	1.28995	-3.23017	1.70761
C	0.57634	-4.40631	1.38511
C	1.24303	-5.64096	1.29443
C	2.63150	-5.71425	1.51876
C	3.34816	-4.54330	1.82722
C	2.68349	-3.30630	1.91712
C	1.32011	-0.67637	3.24987
C	1.69697	3.05483	2.08720
C	2.66522	3.25655	1.08602
C	3.64875	4.25411	1.23696
C	3.67234	5.05614	2.39255
C	2.70460	4.85857	3.39837
C	1.72216	3.86478	3.24689
C	-1.20096	2.67354	2.34348
C	-1.35708	3.98953	1.85776
C	-2.51167	4.73253	2.16246
C	-3.52645	4.17333	2.96146
C	-3.38442	2.85542	3.43600
C	-2.23571	2.10566	3.11864
C	0.66291	0.68209	3.52948
C	2.37390	-0.06231	0.20589
C	3.61071	-0.20396	0.41447
C	4.99784	-0.33066	0.65752
C	5.77497	-1.33350	-0.00596
C	7.14095	-1.45377	0.24137
C	7.79312	-0.57719	1.15728
C	7.02588	0.42492	1.82050
C	5.65936	0.54495	1.57837
C	-1.63211	0.31934	-0.20836
C	-2.84937	0.54394	-0.40872
C	-4.17381	0.94011	-0.65823
C	-5.13618	1.45502	0.30321
C	-6.34178	1.81544	-0.39020
C	-6.18106	1.45616	-1.78335
C	-4.87816	0.86422	-1.93470

Fe	-6.12807	-0.28953	-0.59643
C	-5.95707	-2.27455	0.31332
C	-6.13300	-2.37463	-1.11299
C	-7.42076	-1.79967	-1.44140
C	-8.03500	-1.35583	-0.21642
C	-7.12413	-1.63388	0.86095
C	9.19270	-0.70008	1.40614
C	10.39479	-0.80423	1.61964
H	-1.80840	-2.41516	-0.14561
H	-3.47854	-4.25012	-0.32432
H	-3.55872	-5.67855	-2.37274
H	-1.92364	-5.28269	-4.22190
H	-0.21113	-3.51235	-4.01359
H	1.34221	-4.30399	-1.41455
H	3.38492	-5.56913	-1.97322
H	5.24195	-4.47652	-3.24519
H	5.03882	-2.06834	-3.89608
H	3.02998	-0.78280	-3.30748
H	1.12662	-0.32556	-4.00869
H	-0.45724	-1.08037	-4.20298
H	-2.43652	2.70678	-2.27313
H	-3.53773	4.91539	-2.16297
H	-2.21960	6.95665	-1.58455
H	0.22844	6.75440	-1.11048
H	1.34465	4.55530	-1.23694
H	3.40146	1.22863	-1.58087
H	5.39416	1.90535	-2.88838
H	5.13978	3.35784	-4.90738
H	2.86437	4.13709	-5.59073
H	0.87800	3.49873	-4.26922
H	-1.54706	0.74059	-2.92008
H	-0.52173	1.49293	-4.16568
H	-2.54945	-0.82676	1.75174
H	-4.51578	-1.40873	3.16057
H	-4.27979	-3.04505	5.03474
H	-2.05057	-4.07154	5.50501
H	-0.08993	-3.48705	4.11879
H	-0.49782	-4.37543	1.22889
H	0.67888	-6.54038	1.06218
H	3.14463	-6.67068	1.46388
H	4.41896	-4.58987	2.00630
H	3.26119	-2.42069	2.15928
H	1.31665	-1.29842	4.15191
H	2.35260	-0.54838	2.91743
H	2.66683	2.63791	0.19709
H	4.38976	4.40142	0.45522
H	4.42995	5.82656	2.50916
H	2.71204	5.47708	4.29179
H	0.97169	3.74177	4.02447
H	-0.57851	4.45078	1.25942
H	-2.60713	5.74826	1.78859
H	-4.40412	4.75929	3.22216
H	-4.14987	2.41875	4.07382
H	-2.16463	1.09184	3.49980
H	1.29366	1.27770	4.19665
H	-0.30059	0.54048	4.02571
H	5.28165	-2.00173	-0.70505

H	7.72627	-2.21715	-0.26231
H	7.52274	1.09303	2.51735
H	5.07885	1.31356	2.08093
H	-4.92083	1.62969	1.34781
H	-7.20340	2.30091	0.04676
H	-6.89972	1.62389	-2.57347
H	-4.44944	0.49295	-2.85534
H	-5.10022	-2.61566	0.87731
H	-5.44059	-2.82775	-1.80841
H	-7.86251	-1.74994	-2.42719
H	-9.00585	-0.88791	-0.12266
H	-7.29839	-1.41296	1.90562
H	11.44264	-0.89450	1.80627

Figure S9. SOMO of complex $\mathbf{3}^{2+}$ (-9.75 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

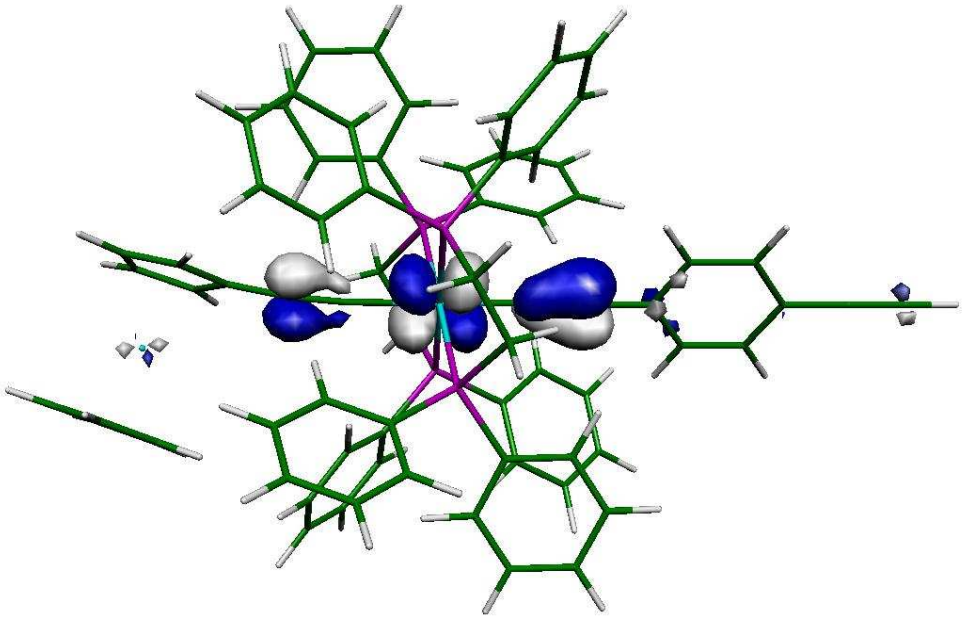


Figure S10. SOMO-1 of complex $\mathbf{3}^{2+}$ (-9.76 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

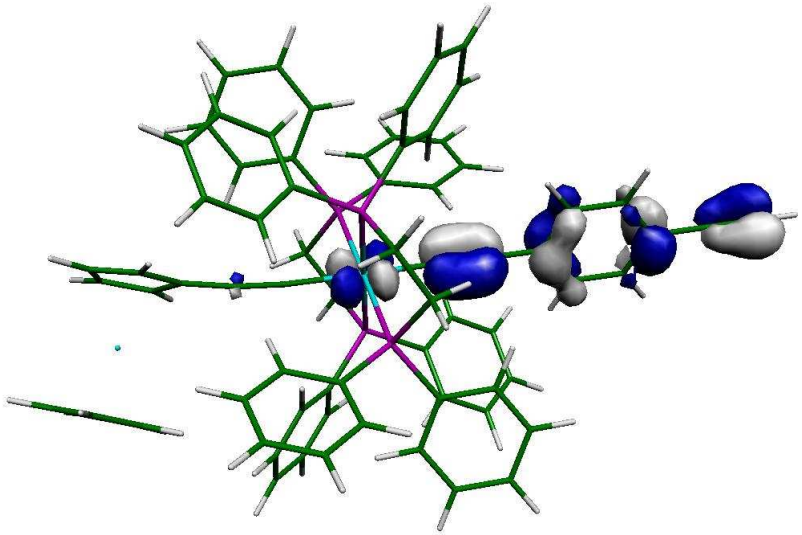
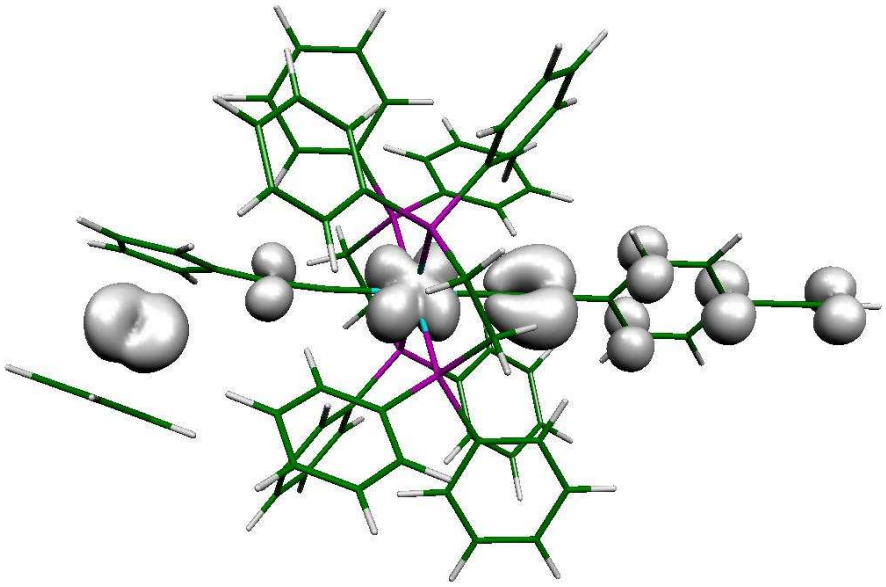


Figure S11. Spin density for complex $\mathbf{3}^{2+}$ shown with a cut-off of 0.002 e/Bohr^3.



Geometry Optimization of Complex Si-3

Input file:

```
%chk=F3SiHSP

#B3LYP/LanL2DZ opt

F3SiHSP

  0  1
```

Cartesians Coordinates for the Optimized Geometry of Complex **Si-3** (-3148.4760236 Hartrees)

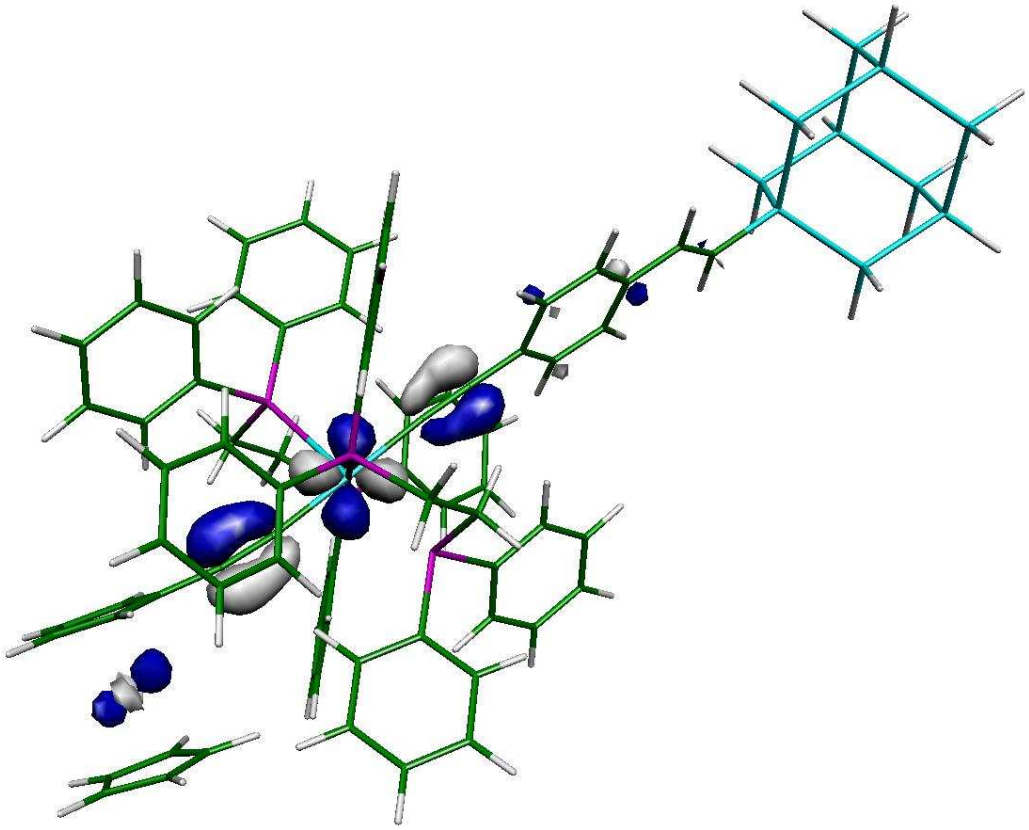
Ru	2.50709	0.22229	0.08728
P	2.43151	-1.27541	2.04973
P	2.95635	1.93773	1.82597
C	3.52593	-2.81606	2.17122
C	4.38148	-3.18126	1.11581
C	5.20078	-4.32254	1.22527
C	5.17689	-5.10464	2.39380
C	4.33174	-4.73653	3.46030
C	3.51232	-3.59998	3.34842
C	0.77933	-1.94700	2.68905
C	0.39321	-3.28107	2.44150
C	-0.84247	-3.76809	2.90600
C	-1.71411	-2.92696	3.62213
C	-1.34683	-1.58711	3.85008
C	-0.11528	-1.09950	3.37777
C	3.04411	-0.27067	3.57864
C	4.08801	3.41691	1.51424
C	5.49202	3.28060	1.53266
C	6.31884	4.39755	1.30875
C	5.75516	5.66108	1.05343
C	4.35365	5.80035	1.01690
C	3.52657	4.68564	1.24357
C	1.62228	2.76049	2.90366
C	0.24987	2.53149	2.68167
C	-0.71720	3.13193	3.51461
C	-0.32271	3.96036	4.57992
C	1.04956	4.18980	4.81014
C	2.01315	3.59625	3.97719
C	3.88134	0.95055	3.16886
P	2.02104	-1.47460	-1.64321
P	2.60548	1.71775	-1.87775
C	3.32705	-2.29289	-2.75237
C	4.69761	-2.00760	-2.59587
C	5.64273	-2.57176	-3.47856
C	5.22986	-3.42101	-4.51949
C	3.85929	-3.71095	-4.67820
C	2.91584	-3.14975	-3.80122
C	0.87693	-2.93949	-1.31676
C	1.42586	-4.21315	-1.04567
C	0.58792	-5.31805	-0.81085
C	-0.81188	-5.16339	-0.83844
C	-1.36343	-3.89433	-1.09290
C	-0.52583	-2.78751	-1.32608
C	1.08767	-0.47195	-2.97045

C	1.54790	3.28664	-1.99420
C	0.66283	3.64073	-0.95941
C	-0.14335	4.79108	-1.07130
C	-0.07612	5.59488	-2.22377
C	0.80263	5.24116	-3.26786
C	1.60812	4.09470	-3.15316
C	4.27042	2.35580	-2.52026
C	4.72002	3.64452	-2.16162
C	5.96342	4.12263	-2.61231
C	6.78133	3.31838	-3.42741
C	6.34973	2.02376	-3.77139
C	5.10956	1.54326	-3.31223
C	1.94115	0.73239	-3.39746
C	0.44491	0.39272	0.08264
C	-0.80067	0.44400	0.00553
C	-2.22988	0.47622	-0.07436
C	-3.02343	-0.54097	0.53701
C	-4.41816	-0.52384	0.45308
C	-5.10288	0.50749	-0.24269
C	-4.31637	1.52281	-0.84536
C	-2.91761	1.51136	-0.76832
C	4.58478	0.06077	0.11489
C	5.82507	0.05868	0.24679
C	7.22201	0.21703	0.49755
C	8.19634	0.85070	-0.37203
C	9.46213	0.90812	0.31479
C	9.29784	0.28217	1.60625
C	7.92969	-0.16259	1.71050
Fe	8.89750	-1.10398	0.08454
C	8.21775	-2.88828	-0.83245
C	8.89026	-3.19817	0.40558
C	10.24975	-2.72514	0.30638
C	10.41828	-2.12056	-0.99342
C	9.16228	-2.22085	-1.69671
C	-6.57053	0.57001	-0.36511
C	-7.48050	-0.33596	0.09157
H	4.43000	-2.56036	0.22944
H	5.85400	-4.59657	0.40046
H	5.80866	-5.98627	2.47620
H	4.30729	-5.33216	4.36995
H	2.85169	-3.33904	4.17218
H	1.04891	-3.94921	1.89291
H	-1.11863	-4.80024	2.70418
H	-2.66517	-3.30521	3.99003
H	-2.01807	-0.91820	4.38342
H	0.12681	-0.05476	3.54367
H	2.16563	0.03971	4.15293
H	3.63294	-0.94783	4.20584
H	5.95121	2.31475	1.70576
H	7.39840	4.27062	1.32646
H	6.39602	6.52415	0.88694
H	3.90340	6.77020	0.81825
H	2.44827	4.81513	1.22344
H	-0.06590	1.88349	1.87060
H	-1.77192	2.94687	3.32466
H	-1.06926	4.42328	5.22138
H	1.36644	4.83092	5.62956

H	3.06614	3.80078	4.15644
H	4.83435	0.63811	2.73682
H	4.07022	1.59993	4.03111
H	5.02429	-1.34708	-1.79698
H	6.69658	-2.34052	-3.35200
H	5.96258	-3.85508	-5.19592
H	3.52846	-4.36990	-5.47761
H	1.86337	-3.39175	-3.92905
H	2.50306	-4.35432	-1.03291
H	1.02844	-6.29258	-0.61311
H	-1.46122	-6.01873	-0.66547
H	-2.44191	-3.75725	-1.10817
H	-0.97380	-1.81578	-1.49995
H	0.87199	-1.11993	-3.82753
H	0.14828	-0.13970	-2.52317
H	0.58255	3.00866	-0.08420
H	-0.82162	5.04978	-0.26144
H	-0.69876	6.48249	-2.31071
H	0.86217	5.85481	-4.16383
H	2.29178	3.84232	-3.96058
H	4.10794	4.28396	-1.53394
H	6.28857	5.11812	-2.32054
H	7.73916	3.69101	-3.78350
H	6.97441	1.38455	-4.39148
H	4.82114	0.53083	-3.57527
H	1.35215	1.42427	-4.00810
H	2.79675	0.40308	-3.99452
H	-2.51834	-1.33410	1.08082
H	-4.98330	-1.31686	0.93741
H	-4.81523	2.32723	-1.38475
H	-2.33731	2.29795	-1.24407
H	7.97338	1.24856	-1.35152
H	10.37491	1.34156	-0.07021
H	10.06516	0.16052	2.35818
H	7.48470	-0.67926	2.54955
H	7.18511	-3.10178	-1.06387
H	8.44493	-3.68140	1.26377
H	11.00652	-2.79971	1.07511
H	11.32282	-1.66275	-1.36959
H	8.96885	-1.85041	-2.69403
H	-6.93597	1.45521	-0.89194
H	-7.11154	-1.22511	0.60888
Si	-9.34987	-0.23013	-0.08707
Si	-10.06894	1.85121	-0.94769
Si	-12.41958	1.90279	-1.12457
Si	-13.14205	0.19466	-2.57873
Si	-12.46993	-1.89755	-1.72909
Si	-13.44132	-2.22371	0.39260
Si	-10.12099	-1.94300	-1.52945
Si	-12.71846	-0.52006	1.85087
Si	-13.38545	1.57305	0.99998
Si	-10.36813	-0.56577	2.02339
H	-9.46827	2.08379	-2.28972
H	-9.61209	2.95054	-0.05466
H	-12.84134	3.22638	-1.66268
H	-12.55948	0.40369	-3.93149
H	-14.62356	0.23860	-2.70703

H	-12.91996	-2.97519	-2.65408
H	-13.04374	-3.55186	0.93213
H	-14.92480	-2.20088	0.28324
H	-9.69569	-3.26769	-0.99900
H	-9.50506	-1.77424	-2.87335
H	-13.32560	-0.72389	3.19594
H	-14.86801	1.63025	0.89061
H	-12.95302	2.65520	1.92458
H	-9.92024	0.49237	2.96891
H	-9.93427	-1.87860	2.57658

Figure S12. HOMO of complex **Si3** (-4.54 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.



Geometry Optimization of Complex Si-3$^+$

Input file:

```
%chk=F3SiH1SP

#B3LYP/LanL2DZ opt

F3SiH1SP

  1  2
```

Cartesian Coordinates for the Optimized Geometry of Complex **Si-3$^+$** (-3148.2879439 Hartrees)

Ru	2.52219	0.19737	0.11052
P	2.50269	-1.31874	2.09298
P	2.87300	1.94398	1.90327
C	3.67006	-2.80203	2.16790
C	4.44150	-3.18512	1.05545
C	5.29300	-4.30517	1.13132
C	5.38583	-5.04700	2.32247
C	4.62288	-4.66234	3.44352
C	3.76823	-3.54946	3.36500
C	0.88546	-2.06926	2.71820
C	0.57683	-3.42166	2.46285
C	-0.62337	-3.98117	2.93754
C	-1.53108	-3.19672	3.67274
C	-1.23865	-1.84016	3.91063
C	-0.04433	-1.27710	3.42610
C	3.06835	-0.28840	3.61636
C	3.93481	3.46701	1.58416
C	5.34269	3.40988	1.65083
C	6.11180	4.56834	1.43253
C	5.48486	5.79235	1.13552
C	4.07960	5.85165	1.05455
C	3.30929	4.69644	1.27598
C	1.49659	2.68577	2.97485
C	0.13498	2.40079	2.75513
C	-0.85193	2.95940	3.59307
C	-0.48670	3.80052	4.65875
C	0.87546	4.08609	4.88471
C	1.86002	3.53510	4.04762
C	3.84811	0.97220	3.21609
P	2.04324	-1.52235	-1.65968
P	2.53592	1.71240	-1.87924
C	3.37548	-2.27944	-2.77357
C	4.73270	-1.92645	-2.64854
C	5.68516	-2.44610	-3.54941
C	5.29202	-3.32127	-4.57649
C	3.93480	-3.68025	-4.70257
C	2.98289	-3.16118	-3.80900
C	0.94837	-3.01230	-1.30834
C	1.53704	-4.27111	-1.05240
C	0.73121	-5.39876	-0.81523
C	-0.67227	-5.28065	-0.82422
C	-1.26190	-4.02608	-1.06457
C	-0.45778	-2.89598	-1.30176
C	1.07109	-0.52409	-2.95538
C	1.42813	3.24228	-1.95917
C	0.53513	3.56057	-0.91920
C	-0.30664	4.68576	-1.02310
C	-0.26476	5.49940	-2.16977
C	0.62439	5.18226	-3.21657
C	1.46492	4.06061	-3.11242
C	4.18092	2.39827	-2.51345
C	4.60656	3.67788	-2.09686
C	5.82613	4.20988	-2.55150
C	6.64119	3.47054	-3.42904
C	6.23235	2.18574	-3.83281
C	5.01631	1.64906	-3.36959
C	1.88904	0.70286	-3.38433

C	0.47630	0.29249	0.12644
C	-0.77039	0.30782	0.04392
C	-2.19726	0.33743	-0.06355
C	-3.01446	-0.51320	0.73696
C	-4.40667	-0.49433	0.61982
C	-5.05695	0.37589	-0.29606
C	-4.24191	1.22548	-1.08888
C	-2.84646	1.20922	-0.98173
C	4.53386	0.12589	0.10498
C	5.78668	0.19300	0.21478
C	7.16199	0.40414	0.42409
C	8.11653	0.98856	-0.51383
C	9.38901	1.09484	0.13948
C	9.26961	0.52155	1.46075
C	7.92109	0.05829	1.62575
Fe	8.84053	-0.95405	0.00319
C	8.27304	-2.82614	-0.89355
C	8.89082	-3.06036	0.38557
C	10.23968	-2.54726	0.32765
C	10.44769	-1.98622	-0.98070
C	9.22738	-2.15143	-1.73499
C	-6.52219	0.43566	-0.46362
C	-7.45812	-0.29828	0.19865
H	4.39168	-2.60767	0.13979
H	5.87252	-4.60218	0.26066
H	6.03870	-5.91461	2.37849
H	4.68465	-5.23068	4.36800
H	3.16440	-3.28579	4.23027
H	1.26607	-4.04805	1.90633
H	-0.84211	-5.02635	2.73495
H	-2.45067	-3.63403	4.05362
H	-1.93442	-1.21973	4.47000
H	0.14032	-0.22230	3.60443
H	2.17706	-0.02161	4.19172
H	3.68777	-0.93666	4.24393
H	5.85231	2.47909	1.87342
H	7.19532	4.50989	1.49578
H	6.08005	6.68827	0.97720
H	3.58306	6.79204	0.82948
H	2.22669	4.76569	1.22590
H	-0.15923	1.74639	1.94312
H	-1.89915	2.73429	3.40707
H	-1.24857	4.23149	5.30342
H	1.16824	4.73845	5.70342
H	2.90342	3.78579	4.22359
H	4.81440	0.70841	2.78067
H	4.01375	1.61664	4.08631
H	5.04741	-1.24790	-1.86239
H	6.72763	-2.15540	-3.45268
H	6.02872	-3.72071	-5.26888
H	3.61999	-4.35868	-5.49122
H	1.94173	-3.45502	-3.91561
H	2.61729	-4.38591	-1.05783
H	1.19842	-6.36337	-0.63323
H	-1.29586	-6.15435	-0.65174
H	-2.34361	-3.92060	-1.06975
H	-0.93686	-1.93898	-1.47479

H	0.86273	-1.17065	-3.81494
H	0.12676	-0.22248	-2.49828
H	0.47480	2.92652	-0.04348
H	-0.99308	4.91762	-0.21250
H	-0.91472	6.36717	-2.24988
H	0.66446	5.80479	-4.10682
H	2.15470	3.83838	-3.92333
H	3.98984	4.27193	-1.43072
H	6.13161	5.19962	-2.22270
H	7.57501	3.89000	-3.79535
H	6.84959	1.60325	-4.51285
H	4.74188	0.64971	-3.69169
H	1.27706	1.37791	-3.99068
H	2.74672	0.39642	-3.98932
H	-2.53397	-1.18654	1.44083
H	-4.99670	-1.16042	1.24372
H	-4.71649	1.90199	-1.79721
H	-2.24355	1.87081	-1.59857
H	7.86220	1.35069	-1.49925
H	10.28567	1.52423	-0.28485
H	10.06139	0.44375	2.19238
H	7.50820	-0.42149	2.50189
H	7.26118	-3.08664	-1.16750
H	8.42807	-3.54015	1.23627
H	10.96448	-2.57527	1.12940
H	11.35578	-1.51950	-1.33634
H	9.07470	-1.83971	-2.75889
H	-6.85663	1.15802	-1.21101
H	-7.11892	-1.02039	0.94622
Si	-9.32821	-0.20750	-0.04466
Si	-9.94440	1.38529	-1.67821
Si	-12.28841	1.42970	-1.91939
Si	-13.04524	-0.69644	-2.59806
Si	-12.47433	-2.29365	-0.96258
Si	-13.47770	-1.71786	1.09002
Si	-10.13156	-2.33305	-0.70722
Si	-12.70966	0.40450	1.76661
Si	-13.27902	2.01000	0.13855
Si	-10.36543	0.35124	2.00797
H	-9.30465	1.03968	-2.97716
H	-9.44658	2.72984	-1.27778
H	-12.64490	2.44215	-2.95117
H	-12.41950	-1.05928	-3.89718
H	-14.51980	-0.66732	-2.78360
H	-12.94294	-3.64000	-1.39189
H	-13.13135	-2.73101	2.12175
H	-14.95624	-1.69400	0.93862
H	-9.74476	-3.34099	0.31811
H	-9.48519	-2.72063	-1.99000
H	-13.32761	0.77212	3.07022
H	-14.75601	2.07143	-0.01738
H	-12.79944	3.35154	0.56423
H	-9.86882	1.67831	2.46154
H	-9.97955	-0.65361	3.03659

Figure S13. SOMO of complex **Si-3**$^{+}$ (-7.15 eV) shown with a cutoff of 0.05 [e/Bohr^{3}]$^{1/2}$.

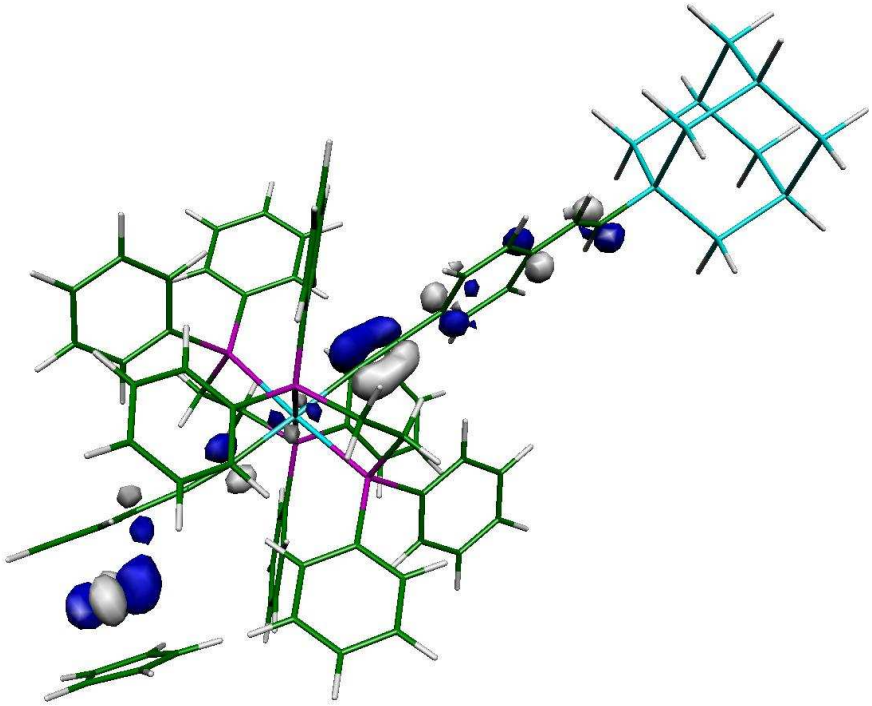
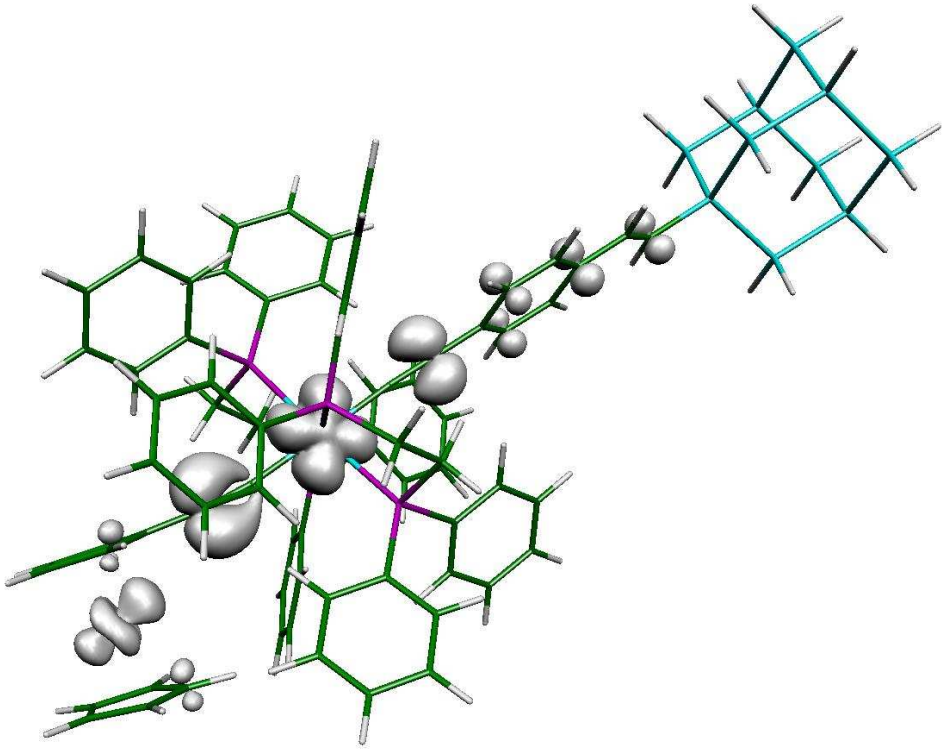


Figure S14. Spin density for complex **Si-3**$^{+}$ shown with a cut-off of 0.002 e/Bohr^{3}.



Geometry Optimization of Complex Si-3^{2+}

Input file:

```
%chk= F3SiH2

#B3LYP/LanL2DZ opt

F3SiH2

  2  3
```

Cartesians Coordinates for the Optimized Geometry of Complex **Si-3^{2+}** (-3148.0163952 Hartrees)

Ru	-4.02296	1.00226	0.03321
P	-3.87390	-0.73093	-1.76620
P	-4.23809	2.54675	-1.95887
C	-5.06253	-2.19796	-1.77314
C	-5.90693	-2.46246	-0.67918
C	-6.75890	-3.58484	-0.69288
C	-6.78246	-4.44527	-1.80582
C	-5.94927	-4.17682	-2.91075
C	-5.09121	-3.06363	-2.89165
C	-2.22338	-1.55665	-2.16592
C	-1.96317	-2.88008	-1.75257
C	-0.73725	-3.49599	-2.06544
C	0.24406	-2.79690	-2.79268
C	-0.00201	-1.46775	-3.18745
C	-1.22334	-0.84795	-2.86750
C	-4.29284	0.13786	-3.42955
C	-5.30391	4.09797	-1.91058
C	-6.69499	4.04575	-2.13890
C	-7.46035	5.22701	-2.13942
C	-6.84702	6.47091	-1.90240
C	-5.45987	6.52736	-1.66379
C	-4.69305	5.34894	-1.66662
C	-2.76165	3.15423	-2.97910
C	-1.42803	2.88716	-2.61656
C	-0.36562	3.34058	-3.42446
C	-0.62828	4.05886	-4.60423
C	-1.96206	4.32682	-4.97356
C	-3.02174	3.88080	-4.16614
C	-5.10118	1.42856	-3.23391
P	-3.78180	-0.53976	2.02227
P	-4.18925	2.73539	1.84178
C	-5.23129	-1.15710	3.07363
C	-6.55896	-0.77450	2.80152
C	-7.60382	-1.18581	3.65442
C	-7.33317	-1.98210	4.78122
C	-6.00617	-2.37045	5.05424
C	-4.96207	-1.95947	4.20808
C	-2.68905	-2.07125	1.94931
C	-3.27167	-3.33656	1.71218
C	-2.47564	-4.49526	1.69336
C	-1.08624	-4.40377	1.90491
C	-0.50029	-3.14490	2.13054
C	-1.29518	-1.98367	2.14941
C	-2.90804	0.58744	3.28471

C	-3.04973	4.24069	1.85176
C	-2.11248	4.46081	0.82551
C	-1.25692	5.57948	0.87054
C	-1.32978	6.48376	1.94596
C	-2.26476	6.26584	2.97810
C	-3.12034	5.15165	2.93146
C	-5.86631	3.51242	2.24508
C	-6.21211	4.75295	1.66725
C	-7.44713	5.35936	1.95864
C	-8.35563	4.73659	2.83498
C	-8.02439	3.49103	3.40170
C	-6.79383	2.87715	3.09934
C	-3.71711	1.87509	3.49624
C	-2.03242	1.05921	0.17536
C	-0.78120	1.04093	0.34876
C	0.61270	1.01199	0.54881
C	1.39166	-0.12685	0.14730
C	2.76311	-0.16444	0.35846
C	3.44792	0.92799	0.97953
C	2.67282	2.06418	1.37058
C	1.29805	2.11067	1.16674
C	-6.06537	0.95544	-0.12033
C	-7.30463	1.01485	-0.31006
C	-8.66380	1.22584	-0.58215
C	-9.67435	1.76108	0.31876
C	-10.91558	1.88953	-0.39452
C	-10.72440	1.35291	-1.72523
C	-9.36552	0.88762	-1.81758
Fe	-10.47945	-0.18464	-0.30414
C	-10.04453	-2.04942	0.78526
C	-10.34153	-2.31607	-0.59737
C	-11.69736	-1.87615	-0.85334
C	-12.22922	-1.34172	0.37478
C	-11.20164	-1.43524	1.37849
C	4.88712	0.93850	1.23014
C	5.77011	-0.07724	0.96692
H	-5.90538	-1.79837	0.17758
H	-7.38122	-3.80114	0.17274
H	-7.42872	-5.31953	-1.81120
H	-5.95512	-4.83846	-3.77274
H	-4.42932	-2.89457	-3.73772
H	-2.70876	-3.44309	-1.20105
H	-0.55764	-4.52016	-1.74944
H	1.18168	-3.28083	-3.05359
H	0.74861	-0.91564	-3.74714
H	-1.37689	0.18197	-3.17487
H	-3.35183	0.35025	-3.94492
H	-4.85281	-0.57300	-4.04502
H	-7.19037	3.10014	-2.33133
H	-8.52865	5.17569	-2.33370
H	-7.43670	7.38378	-1.91640
H	-4.97358	7.48347	-1.48950
H	-3.62172	5.41689	-1.50296
H	-1.20894	2.32854	-1.71464
H	0.65961	3.13170	-3.12955
H	0.19058	4.40928	-5.22687
H	-2.17515	4.88508	-5.88119

H	-4.04200	4.11825	-4.45730
H	-6.10229	1.20579	-2.85808
H	-5.18968	1.97415	-4.17958
H	-6.77775	-0.15642	1.93799
H	-8.62288	-0.86428	3.44960
H	-8.13841	-2.29532	5.44062
H	-5.78564	-2.98680	5.92148
H	-3.94663	-2.27647	4.43085
H	-4.34368	-3.43228	1.56687
H	-2.94031	-5.46352	1.52624
H	-0.47277	-5.30090	1.90437
H	0.56969	-3.06339	2.30305
H	-0.81650	-1.02780	2.33234
H	-2.80103	0.04078	4.22819
H	-1.91257	0.81532	2.89683
H	-2.03796	3.76398	-0.00015
H	-0.54187	5.74255	0.06782
H	-0.67168	7.34802	1.98072
H	-2.33023	6.96099	3.81082
H	-3.84827	5.00987	3.72699
H	-5.52057	5.26275	1.00496
H	-7.68847	6.32007	1.51205
H	-9.29714	5.22002	3.08309
H	-8.70742	3.00749	4.09661
H	-6.57746	1.91460	3.55171
H	-3.13887	2.59412	4.08479
H	-4.63565	1.65929	4.04819
H	0.88429	-0.95950	-0.33034
H	3.32252	-1.03888	0.04032
H	3.17685	2.90468	1.84205
H	0.72364	2.97988	1.47522
H	-9.47414	2.10330	1.32444
H	-11.82254	2.33743	-0.01275
H	-11.46061	1.32857	-2.51660
H	-8.90322	0.43599	-2.68452
H	-9.10985	-2.25445	1.28813
H	-9.67883	-2.78741	-1.30968
H	-12.23076	-1.97098	-1.78914
H	-13.22383	-0.94197	0.51915
H	-11.29567	-1.11292	2.40690
H	5.26841	1.85675	1.67852
H	5.37762	-0.99855	0.52690
Si	7.63102	-0.08256	1.29879
Si	8.45423	2.01597	2.00184
Si	10.77608	1.85334	2.37863
Si	11.17566	0.25955	4.06843
Si	10.38337	-1.84693	3.36988
Si	11.46680	-2.51036	1.38553
Si	8.06374	-1.71114	2.96968
Si	11.05561	-0.90891	-0.29307
Si	11.84757	1.20540	0.38113
Si	8.73509	-0.77005	-0.68237
H	7.74402	2.42891	3.24318
H	8.15341	3.02753	0.95289
H	11.27051	3.18798	2.81113
H	10.48027	0.66775	5.31661
H	12.63333	0.17670	4.33949

H	10.60973	-2.85584	4.43965
H	10.95030	-3.83447	0.95228
H	12.92800	-2.62208	1.62479
H	7.52388	-3.01684	2.50285
H	7.32685	-1.32341	4.20190
H	11.71641	-1.31678	-1.56197
H	13.31429	1.14151	0.60431
H	11.56950	2.20542	-0.68214
H	8.43052	0.21035	-1.75826
H	8.17840	-2.08837	-1.09111

Figure S15. SOMO of complex **Si-3**$^{2+}$ (-9.39 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

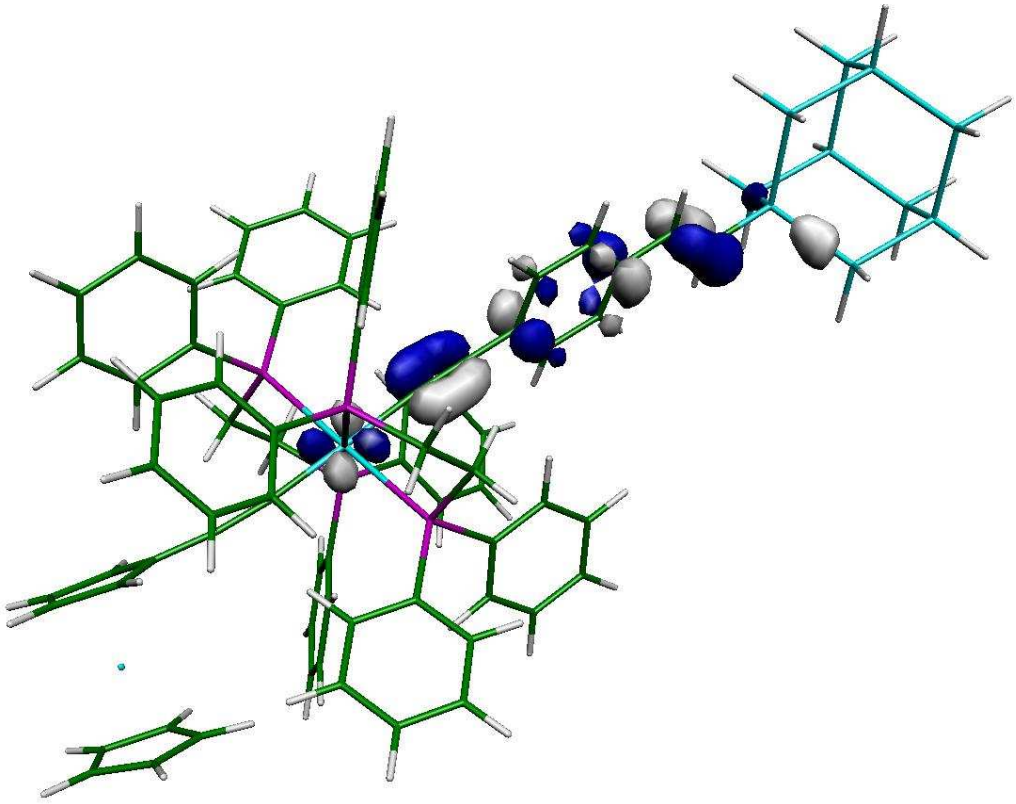


Figure S16. SOMO-1 of complex **Si-3**$^{2+}$ (-9.49 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

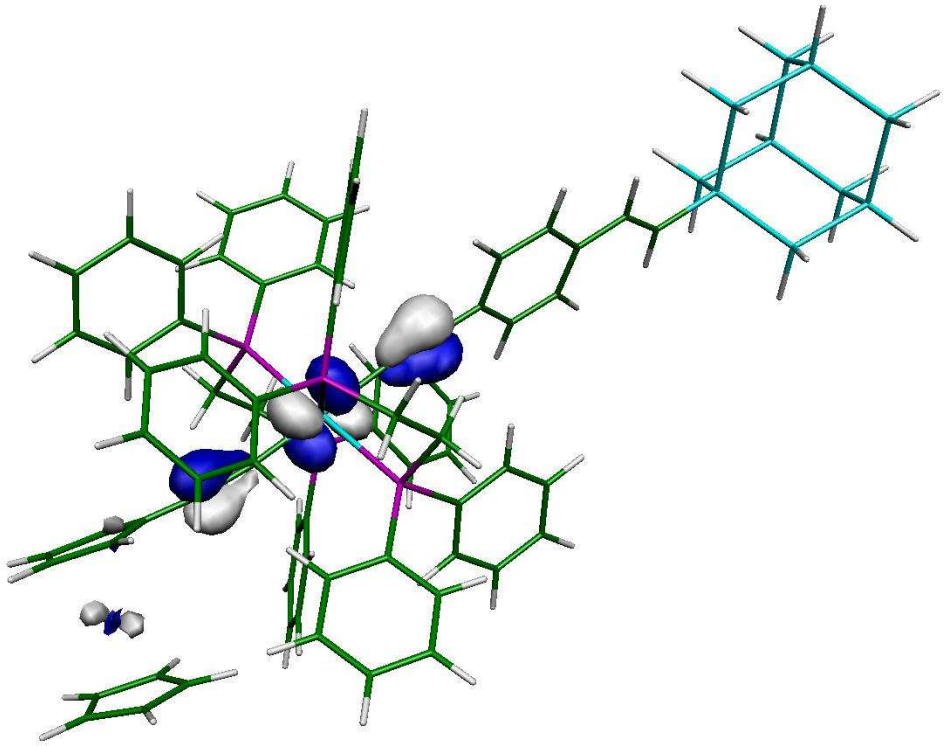
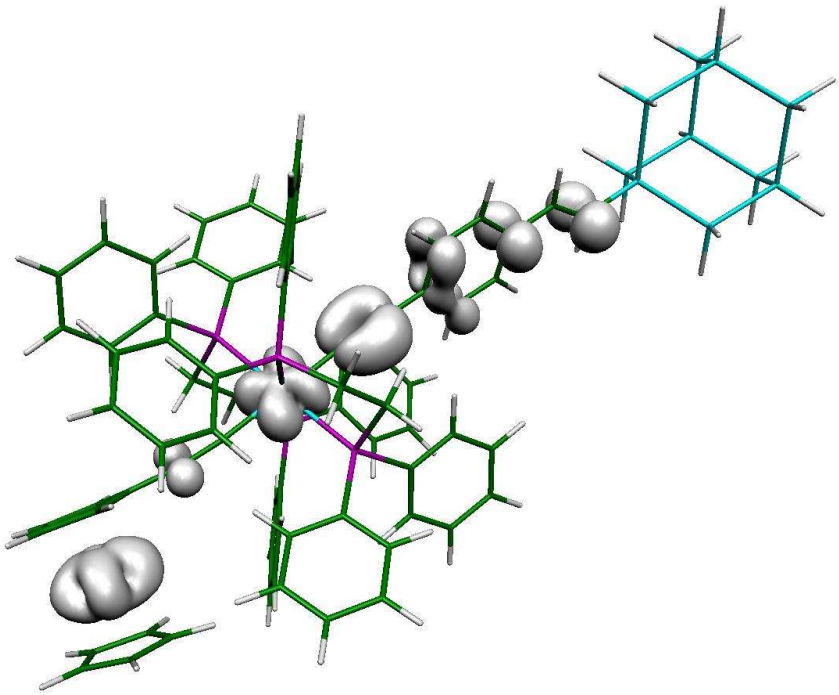


Figure S17. Spin density for complex **Si-3**$^{2+}$ shown with a cut-off of 0.002 e/Bohr^3.



Geometry Optimization of Complex 4

Input file:

```
%chk=FedP4de3SPSP

#B3LYP/LanL2DZ opt

FedP4de3SPSP

  0  1
```

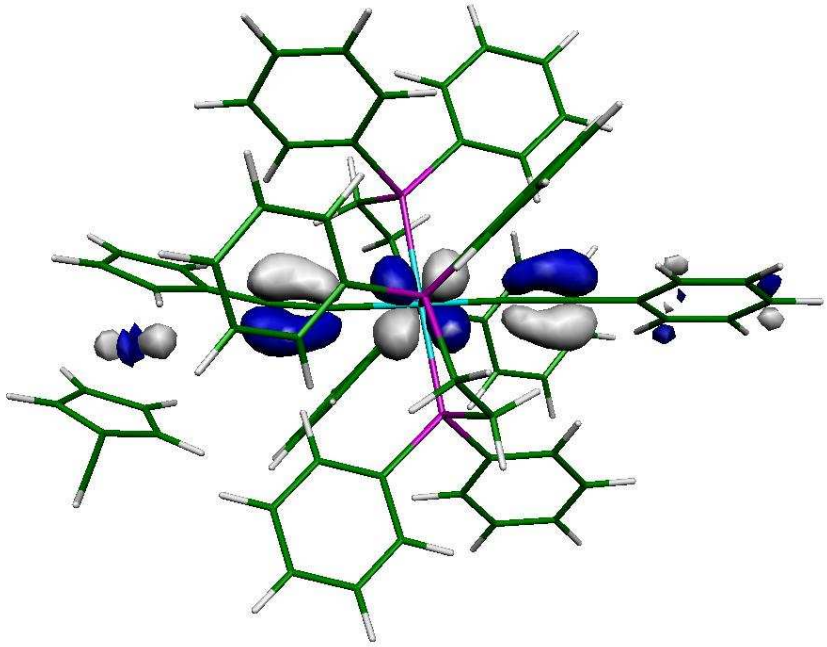
Cartesian Coordinates for the Optimized Geometry of Complex **4** (`-3099.9343658 Hartrees`)

Ru	0.69949	0.07698	0.04861
P	0.79851	-1.51750	-1.82931
P	0.85637	1.74253	-1.78588
C	-0.52374	-2.85257	-2.06633
C	-1.56280	-3.01308	-1.13140
C	-2.53944	-4.01198	-1.31532
C	-2.49212	-4.85291	-2.44158
C	-1.46271	-4.68734	-3.39042
C	-0.48533	-3.69454	-3.20215
C	2.37885	-2.50193	-2.18151
C	2.47786	-3.86356	-1.82653
C	3.65948	-4.58555	-2.07523
C	4.76280	-3.95610	-2.68054
C	4.68029	-2.59088	-3.01405
C	3.50188	-1.86806	-2.75601
C	0.61222	-0.51295	-3.46625
C	-0.00823	3.41931	-1.70479
C	-1.39140	3.54418	-1.95264
C	-2.01321	4.80585	-1.89948
C	-1.26506	5.95585	-1.58764
C	0.11293	5.83523	-1.32121
C	0.73561	4.57553	-1.37685
C	2.46814	2.24442	-2.66315
C	3.72516	1.79546	-2.21270
C	4.90123	2.16145	-2.90018
C	4.83191	2.97307	-4.04618
C	3.57610	3.42253	-4.50434
C	2.40490	3.06286	-3.81631
C	-0.02693	0.86415	-3.23120
P	0.58996	-1.58126	1.87854
P	0.59510	1.68349	1.92233
C	-0.99801	-2.11453	2.77453
C	-2.25697	-1.60357	2.40160
C	-3.41012	-1.94864	3.13811
C	-3.31519	-2.80915	4.24576
C	-2.05905	-3.32851	4.61945
C	-0.90941	-2.98105	3.89010
C	1.50546	-3.22882	1.78612
C	0.79785	-4.40867	1.46256
C	1.46162	-5.64703	1.40058
C	2.84504	-5.72181	1.65488
C	3.55767	-4.54762	1.96023
C	2.89476	-3.30741	2.02060
C	1.45255	-0.67774	3.32224

C	1.92454	3.00929	2.17922
C	2.98969	3.15353	1.27149
C	3.98397	4.12895	1.48507
C	3.92513	4.96668	2.61342
C	2.86439	4.82343	3.53090
C	1.87223	3.85120	3.31448
C	-0.98275	2.67835	2.24936
C	-1.07251	4.03274	1.86508
C	-2.25474	4.76305	2.08310
C	-3.36824	4.14945	2.68577
C	-3.29356	2.79239	3.05216
C	-2.11348	2.06129	2.82613
C	0.76692	0.67697	3.55738
C	2.73504	-0.12323	0.38098
C	3.94234	-0.27081	0.65838
C	5.33436	-0.43731	0.97142
C	6.07748	-1.53794	0.45761
C	7.43828	-1.69802	0.76850
C	8.09800	-0.76924	1.59942
C	7.37559	0.32514	2.11774
C	6.01493	0.49067	1.81021
C	-1.34132	0.29312	-0.30231
C	-2.52594	0.50432	-0.63352
C	-3.80260	0.90307	-1.13129
C	-4.81716	1.67741	-0.44128
C	-5.89043	1.96221	-1.36046
C	-5.57292	1.33753	-2.62356
C	-4.30596	0.66497	-2.47601
Fe	-5.72795	-0.11661	-1.12275
C	-5.60149	-1.93141	-0.04046
C	-5.87810	-2.21282	-1.42236
C	-7.12647	-1.57911	-1.77249
C	-7.62689	-0.89950	-0.60849
C	-6.68830	-1.11798	0.47729
C	-6.83399	-0.63713	1.81197
C	-6.98611	-0.24706	2.96287
H	-1.62477	-2.34504	-0.28089
H	-3.33050	-4.13154	-0.57892
H	-3.24532	-5.62527	-2.58105
H	-1.41711	-5.33058	-4.26620
H	0.31545	-3.59410	-3.93137
H	1.64018	-4.37064	-1.35934
H	3.71328	-5.63399	-1.79207
H	5.67329	-4.51610	-2.88173
H	5.53086	-2.08408	-3.46374
H	3.48087	-0.80981	-2.99600
H	1.60664	-0.40293	-3.90957
H	0.00221	-1.10782	-4.15405
H	-1.99395	2.67152	-2.17396
H	-3.08043	4.88048	-2.09294
H	-1.74686	6.93050	-1.55266
H	0.70351	6.71493	-1.07583
H	1.80143	4.50378	-1.17972
H	3.78881	1.15797	-1.33703
H	5.86245	1.80810	-2.53426
H	5.73940	3.25480	-4.57562
H	3.51035	4.05318	-5.38804

H	1.44690	3.43668	-4.16994
H	-1.07577	0.75980	-2.94579
H	0.04259	1.48423	-4.13223
H	-2.33892	-0.93741	1.54710
H	-4.37379	-1.53354	2.85627
H	-4.20690	-3.07318	4.80974
H	-1.97502	-3.99768	5.47276
H	0.05141	-3.39671	4.18385
H	-0.27153	-4.37186	1.27410
H	0.89863	-6.54598	1.16001
H	3.35850	-6.67999	1.61552
H	4.62812	-4.58728	2.14653
H	3.46872	-2.41281	2.23313
H	1.40111	-1.30180	4.22182
H	2.49815	-0.53837	3.03805
H	3.06062	2.49058	0.41875
H	4.80138	4.22361	0.77402
H	4.69354	5.71853	2.77911
H	2.80838	5.46566	4.40685
H	1.05120	3.76481	4.02270
H	-0.22715	4.52697	1.39751
H	-2.30204	5.80493	1.77575
H	-4.28082	4.71537	2.85931
H	-4.15105	2.29773	3.50304
H	-2.09738	1.00984	3.09348
H	1.34253	1.28224	4.26526
H	-0.23444	0.53268	3.97475
H	5.57232	-2.25352	-0.18527
H	7.98578	-2.54690	0.36306
H	9.15143	-0.89588	1.83897
H	7.87331	1.04767	2.76166
H	5.46159	1.33563	2.21278
H	-4.74547	2.00780	0.58468
H	-6.77747	2.53986	-1.14030
H	-6.18064	1.36004	-3.51770
H	-3.79333	0.08763	-3.23304
H	-4.74266	-2.26064	0.52483
H	-5.24520	-2.78346	-2.08625
H	-7.59990	-1.60074	-2.74396
H	-8.54116	-0.32804	-0.53332
H	-7.12196	0.09773	3.96199

Figure S18. HOMO of complex **4** (-4.41 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.



Geometry Optimization of Complex 4^+

Input file:

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%chk=FedP4de3SPSP1SP

#B3LYP/LanL2DZ opt

FedP4de3SPSP1SP

  1  2
```

Cartesians Coordinates for the Optimized Geometry of Complex **4^+** (-3099.7462635 Hartrees)

Ru	0.67619	0.07651	0.04289
P	0.80469	-1.51521	-1.87902
P	0.90690	1.77028	-1.82495
C	-0.53540	-2.82659	-2.10886
C	-1.54120	-3.02129	-1.14444
C	-2.52141	-4.01630	-1.32884
C	-2.50920	-4.81901	-2.48361
C	-1.51023	-4.62162	-3.45848
C	-0.52828	-3.63365	-3.27060
C	2.37771	-2.51032	-2.20222
C	2.44979	-3.86801	-1.82542
C	3.61646	-4.61513	-2.06820
C	4.72744	-4.01573	-2.68980
C	4.66897	-2.65553	-3.04801

C	3.50648	-1.90483	-2.79578
C	0.64572	-0.48700	-3.49807
C	0.06604	3.45272	-1.72845
C	-1.30677	3.60309	-2.01584
C	-1.90884	4.87394	-1.96194
C	-1.15026	6.00569	-1.61149
C	0.21805	5.85892	-1.31100
C	0.82228	4.59054	-1.36707
C	2.54520	2.22655	-2.66032
C	3.78301	1.73694	-2.20098
C	4.97584	2.08382	-2.86786
C	4.94062	2.91519	-4.00108
C	3.70306	3.40420	-4.46756
C	2.51395	3.06524	-3.80043
C	0.01785	0.89373	-3.26184
P	0.55822	-1.61296	1.90657
P	0.57193	1.67661	1.96394
C	-1.05187	-2.11730	2.76540
C	-2.29355	-1.56096	2.40266
C	-3.45848	-1.89407	3.12472
C	-3.39128	-2.78779	4.20791
C	-2.15151	-3.35025	4.57245
C	-0.98894	-3.01504	3.85806
C	1.46412	-3.25787	1.79272
C	0.75152	-4.42793	1.44615
C	1.40793	-5.66983	1.38471
C	2.78612	-5.75648	1.66198
C	3.50225	-4.59159	1.99321
C	2.84766	-3.34738	2.05487
C	1.41827	-0.70476	3.34164
C	1.91230	2.98608	2.20768
C	2.96908	3.13821	1.29153
C	3.96853	4.10652	1.51101
C	3.92042	4.92917	2.65084
C	2.86508	4.78002	3.57348
C	1.86733	3.81481	3.35329
C	-1.00532	2.67188	2.26501
C	-1.08720	4.01107	1.82735
C	-2.25928	4.75997	2.03479
C	-3.36774	4.18095	2.68000
C	-3.29869	2.84006	3.10271
C	-2.12911	2.08794	2.88832
C	0.73355	0.64852	3.58039
C	2.68091	-0.13828	0.39086
C	3.88273	-0.30441	0.68757
C	5.26473	-0.47037	1.03389
C	6.06582	-1.45639	0.39299
C	7.41557	-1.61710	0.74414
C	7.99757	-0.79780	1.73345
C	7.21555	0.18533	2.37436
C	5.86368	0.34732	2.03334
C	-1.29554	0.30340	-0.30897
C	-2.48061	0.55910	-0.64816
C	-3.73521	0.97422	-1.13901
C	-4.76679	1.71623	-0.42277
C	-5.83090	2.01339	-1.33770
C	-5.51194	1.41550	-2.61424

C	-4.24988	0.74430	-2.48876
Fe	-5.64806	-0.09320	-1.12963
C	-5.62072	-1.95093	-0.05736
C	-5.84558	-2.19760	-1.45410
C	-7.06974	-1.53308	-1.83482
C	-7.59739	-0.86703	-0.67971
C	-6.70173	-1.12169	0.43400
C	-6.88391	-0.65526	1.76945
C	-7.07664	-0.27297	2.91573
H	-1.57187	-2.39452	-0.26102
H	-3.28316	-4.16902	-0.56805
H	-3.26234	-5.59073	-2.62297
H	-1.49001	-5.23867	-4.35307
H	0.25168	-3.51442	-4.01926
H	1.60262	-4.35399	-1.35301
H	3.65138	-5.66088	-1.77427
H	5.62336	-4.59757	-2.89147
H	5.52235	-2.17696	-3.52198
H	3.50380	-0.85330	-3.06487
H	1.64527	-0.38200	-3.92890
H	0.03972	-1.06769	-4.20072
H	-1.91644	2.74825	-2.28512
H	-2.96612	4.97408	-2.19314
H	-1.61501	6.98800	-1.57989
H	0.81617	6.72610	-1.04295
H	1.88231	4.50068	-1.14924
H	3.82170	1.08604	-1.33559
H	5.92410	1.70259	-2.49716
H	5.86100	3.18243	-4.51416
H	3.66507	4.05010	-5.34099
H	1.57188	3.47109	-4.16122
H	-1.03488	0.80022	-2.98768
H	0.09839	1.51378	-4.16145
H	-2.35640	-0.86957	1.56872
H	-4.40968	-1.44496	2.85301
H	-4.29143	-3.04361	4.76105
H	-2.08933	-4.04297	5.40775
H	-0.04201	-3.46340	4.14788
H	-0.31512	-4.38467	1.24593
H	0.84300	-6.56325	1.13077
H	3.29205	-6.71808	1.62605
H	4.56685	-4.64451	2.20521
H	3.42472	-2.46393	2.30362
H	1.36101	-1.33138	4.23862
H	2.46605	-0.56875	3.06634
H	3.03074	2.49431	0.42347
H	4.78130	4.20908	0.79628
H	4.69261	5.67522	2.82102
H	2.81756	5.41232	4.45636
H	1.05026	3.72605	4.06568
H	-0.24223	4.48146	1.33513
H	-2.30049	5.79127	1.69441
H	-4.26858	4.76472	2.85259
H	-4.14795	2.37833	3.60089
H	-2.11610	1.05293	3.21429
H	1.30678	1.24594	4.29622
H	-0.26834	0.50258	3.99392

H	5.61607	-2.08680	-0.36865
H	8.01528	-2.37709	0.24906
H	9.04356	-0.92370	2.00144
H	7.66009	0.81939	3.13745
H	5.26096	1.10681	2.52497
H	-4.69294	2.03537	0.60654
H	-6.72189	2.58109	-1.10932
H	-6.12536	1.45304	-3.50347
H	-3.73391	0.19405	-3.26310
H	-4.79388	-2.31248	0.53588
H	-5.21223	-2.78605	-2.10167
H	-7.51281	-1.53431	-2.82068
H	-8.50400	-0.28131	-0.62577
H	-7.26246	0.05699	3.91276

Figure S19. SOMO of complex $\mathbf{4}^{+}$ (-7.39 eV) shown with a cutoff of 0.05 $[e/Bohr^3]^{1/2}$.

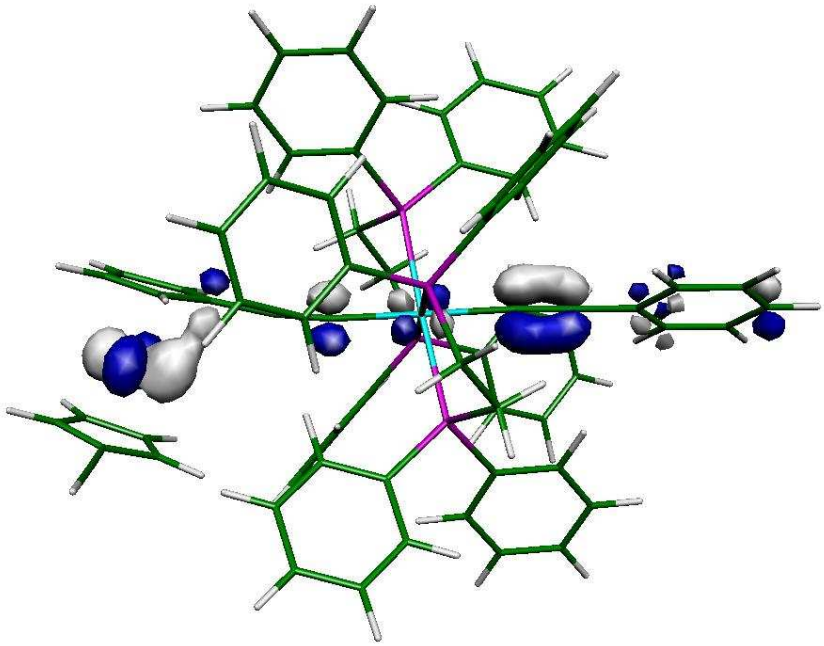
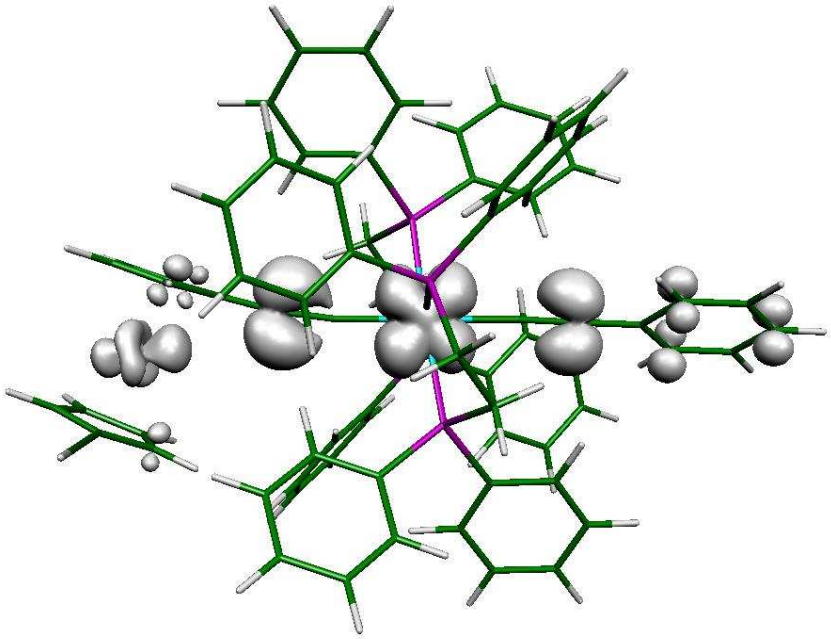


Figure S20. Spin density for complex $\mathbf{4}^{+}$ shown with a cut-off of 0.002 e/Bohr^3.



Geometry Optimization of Complex $\mathbf{4}^{2+}$

Input file:

```
%chk=FedP4de3SPSP2SP

#B3LYP/LanL2DZ opt

FedP4de3SPSP2SP

  2  3
```

Cartesian Coordinates for the Optimized Geometry of Complex $\mathbf{4}^{2+}$ (-3099.4646067Hartrees)

Ru	0.73882	0.08109	0.03960
P	0.84389	-1.51797	-1.88981
P	1.00066	1.77387	-1.83874
C	-0.53558	-2.78594	-2.12640
C	-1.55339	-2.95221	-1.16915
C	-2.55375	-3.92693	-1.35642
C	-2.55222	-4.73425	-2.50871
C	-1.54255	-4.56246	-3.47744
C	-0.53825	-3.59788	-3.28488
C	2.38946	-2.56048	-2.18888
C	2.42343	-3.90515	-1.76145
C	3.56150	-4.69820	-1.99353
C	4.68071	-4.15878	-2.65472
C	4.66026	-2.81183	-3.06399

C	3.52679	-2.01359	-2.82271
C	0.72872	-0.48449	-3.50678
C	0.20438	3.47626	-1.76151
C	-1.14114	3.67770	-2.13440
C	-1.69937	4.96934	-2.11063
C	-0.92347	6.07101	-1.70579
C	0.41763	5.87359	-1.32311
C	0.97825	4.58453	-1.34910
C	2.66744	2.17433	-2.64192
C	3.87932	1.62333	-2.18594
C	5.09036	1.93056	-2.83831
C	5.09747	2.78429	-3.95546
C	3.88515	3.33416	-4.41963
C	2.67780	3.03471	-3.76640
C	0.11437	0.90357	-3.28013
P	0.46978	-1.61600	1.90864
P	0.64962	1.68402	1.97424
C	-1.18277	-2.03599	2.73039
C	-2.38532	-1.40827	2.35166
C	-3.58112	-1.69066	3.04384
C	-3.58504	-2.60114	4.11562
C	-2.38395	-3.23151	4.49754
C	-1.19022	-2.94960	3.81153
C	1.30101	-3.30034	1.80612
C	0.54574	-4.43755	1.44128
C	1.14835	-5.70721	1.39581
C	2.51375	-5.85488	1.70802
C	3.27233	-4.72306	2.05927
C	2.67201	-3.45129	2.10463
C	1.35783	-0.75048	3.35335
C	2.02770	2.94852	2.22730
C	3.08333	3.08657	1.30669
C	4.10952	4.02427	1.53576
C	4.08838	4.83021	2.68855
C	3.03291	4.69672	3.61348
C	2.00825	3.76220	3.38459
C	-0.90148	2.72530	2.26255
C	-0.94499	4.05371	1.78748
C	-2.08130	4.85385	2.00334
C	-3.19069	4.33928	2.70003
C	-3.16025	3.00962	3.16212
C	-2.02857	2.20378	2.93462
C	0.75711	0.64178	3.58647
C	2.67419	-0.19941	0.40583
C	3.87766	-0.41477	0.71629
C	5.23284	-0.63061	1.07818
C	6.03069	-1.59237	0.38402
C	7.36383	-1.80363	0.75560
C	7.93223	-1.06250	1.81623
C	7.15744	-0.10509	2.50972
C	5.82189	0.10980	2.15077
C	-1.26139	0.39677	-0.33513
C	-2.44091	0.69044	-0.64163
C	-3.71299	1.16131	-1.01107
C	-4.72809	1.73283	-0.14018
C	-5.84298	2.15713	-0.93934
C	-5.57408	1.78807	-2.31419

C	-4.29587	1.12956	-2.34873
Fe	-5.72780	0.04174	-1.13186
C	-5.75375	-1.93275	-0.19226
C	-5.77760	-2.04569	-1.62361
C	-6.99130	-1.41613	-2.10063
C	-7.71699	-0.92555	-0.96360
C	-6.95657	-1.24142	0.22538
C	-7.32843	-0.91860	1.55990
C	-7.69067	-0.66746	2.70036
H	-1.57081	-2.32840	-0.28274
H	-3.31367	-4.07415	-0.59187
H	-3.31520	-5.49622	-2.64714
H	-1.52801	-5.18557	-4.36751
H	0.25206	-3.50450	-4.02608
H	1.56773	-4.34760	-1.26216
H	3.56656	-5.73427	-1.66621
H	5.55118	-4.77849	-2.85334
H	5.51721	-2.38324	-3.57734
H	3.55313	-0.97597	-3.14078
H	1.73652	-0.38940	-3.91910
H	0.13089	-1.05573	-4.22389
H	-1.75703	2.84606	-2.45957
H	-2.73217	5.11505	-2.41671
H	-1.35160	7.06991	-1.70135
H	1.02950	6.71857	-1.01897
H	2.02045	4.45738	-1.07227
H	3.88802	0.95544	-1.33346
H	6.02015	1.50340	-2.47147
H	6.03134	3.02202	-4.45772
H	3.88085	3.99687	-5.28074
H	1.75719	3.48716	-4.12651
H	-0.94316	0.82312	-3.01935
H	0.21499	1.52092	-4.17951
H	-2.39202	-0.70079	1.53018
H	-4.50241	-1.18627	2.76116
H	-4.50690	-2.81698	4.64924
H	-2.37564	-3.93537	5.32521
H	-0.27578	-3.45178	4.11616
H	-0.51287	-4.34923	1.21615
H	0.55149	-6.57559	1.12966
H	2.97616	-6.83815	1.68750
H	4.32576	-4.82629	2.30479
H	3.28159	-2.59770	2.38107
H	1.25165	-1.37178	4.24947
H	2.41732	-0.67955	3.09853
H	3.12094	2.46354	0.42152
H	4.91986	4.12038	0.81753
H	4.87997	5.55346	2.86561
H	3.00602	5.31823	4.50444
H	1.19211	3.68781	4.09972
H	-0.09370	4.47974	1.26712
H	-2.09000	5.87793	1.64032
H	-4.05645	4.96781	2.89242
H	-4.00167	2.60570	3.72082
H	-2.04398	1.18278	3.30266
H	1.36775	1.20412	4.29956
H	-0.24783	0.55591	4.00770

H	5.58471	-2.15951	-0.42751
H	7.96513	-2.53876	0.22808
H	8.96818	-1.22876	2.09957
H	7.60076	0.46339	3.32226
H	5.22161	0.84924	2.67400
H	-4.60541	1.88639	0.92266
H	-6.71389	2.68846	-0.58126
H	-6.20697	1.99489	-3.16610
H	-3.80670	0.73123	-3.22699
H	-4.99220	-2.30964	0.47550
H	-5.03443	-2.54325	-2.23008
H	-7.31882	-1.36332	-3.12960
H	-8.66994	-0.41407	-0.97440
H	-8.02407	-0.45217	3.69248

Figure S21. SOMO of complex $\mathbf{4}^{2+}$ (-9.84 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

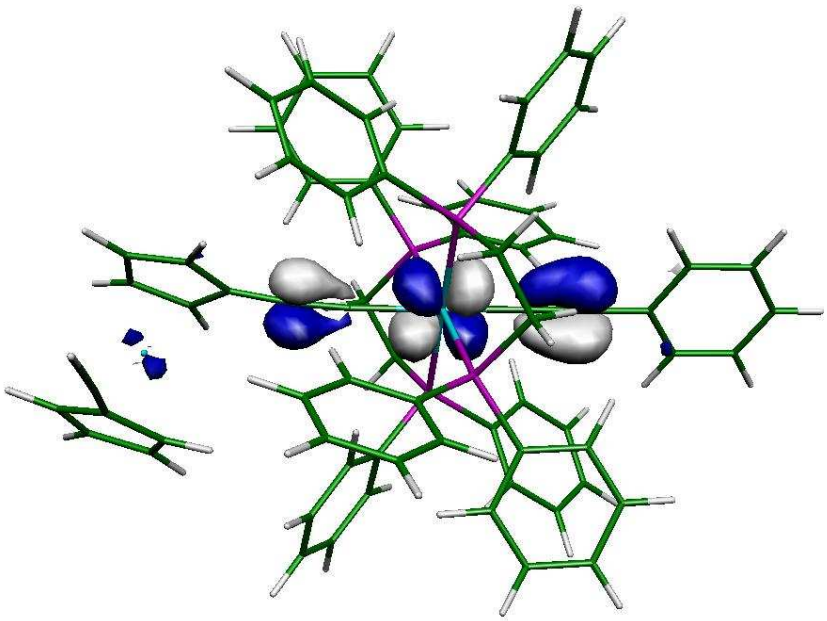


Figure S22. SOMO-1 of complex $\mathbf{4}^{2+}$ (-9.96 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

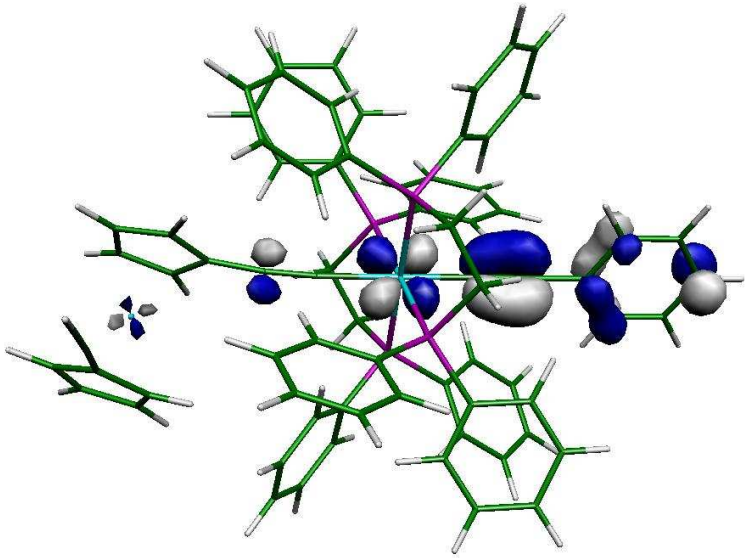
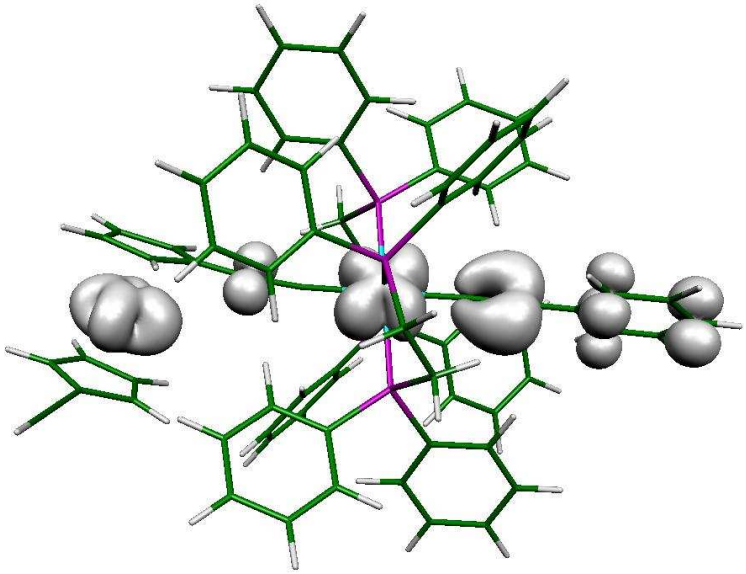


Figure S23. Spin density for complex $\mathbf{4}^{2+}$ shown with a cut-off of 0.002 e/Bohr^3.



Geometry Optimization of Complex Si-4

Input file:

```
%chk=F4SiHSP

#B3LYP/LanL2DZ opt

F4SiHSP

  0  1
```

Cartesian Coordinates for the Optimized Geometry of Complex **Si-4** (-3148.4751224 Hartrees)

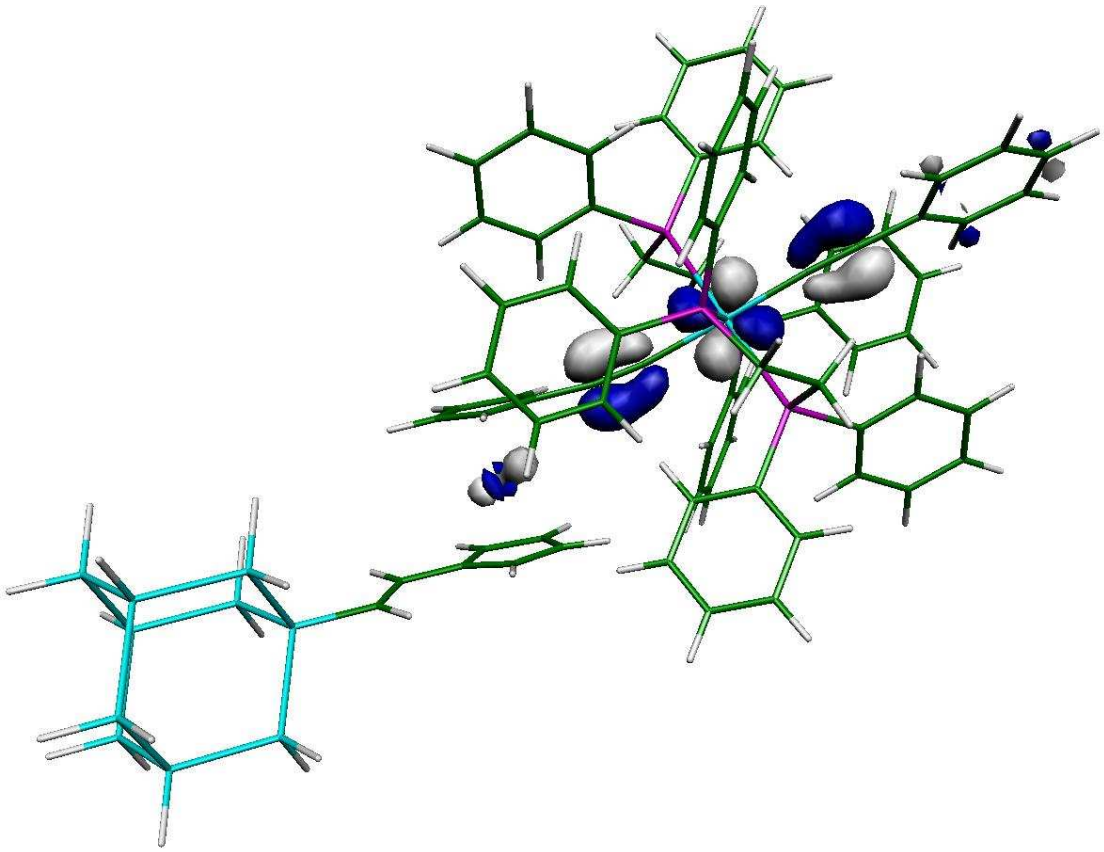
Ru	3.27606	0.13749	0.05253
P	3.93975	-1.49962	-1.66915
P	3.29883	1.69014	-1.88735
C	2.96561	-3.09996	-1.94809
C	1.86323	-3.42672	-1.13706
C	1.13959	-4.61466	-1.36254
C	1.50751	-5.48325	-2.40561
C	2.60308	-5.15553	-3.23006
C	3.32656	-3.97224	-3.00138
C	5.72096	-2.13658	-1.76181
C	6.05633	-3.41774	-1.27589
C	7.38457	-3.87860	-1.32628
C	8.39973	-3.06389	-1.86100
C	8.07643	-1.77475	-2.32527
C	6.74981	-1.31189	-2.26558
C	3.74866	-0.65460	-3.39331
C	2.09531	3.13688	-2.03924
C	0.76198	2.94178	-2.45686
C	-0.11538	4.03634	-2.57369
C	0.32377	5.33691	-2.26532
C	1.64957	5.53631	-1.83230
C	2.52755	4.44372	-1.71751
C	4.86382	2.48306	-2.62384
C	6.12639	2.32383	-2.01914
C	7.27541	2.89350	-2.60623
C	7.17558	3.62166	-3.80484
C	5.91513	3.78190	-4.41677
C	4.76938	3.21875	-3.82957
C	2.80739	0.55828	-3.34172
P	3.30213	-1.39264	1.99131
P	2.59873	1.77604	1.77083
C	1.75926	-2.18720	2.76496
C	0.47937	-1.98852	2.21084
C	-0.65905	-2.52646	2.84745
C	-0.53120	-3.26453	4.03665
C	0.74809	-3.46962	4.59243
C	1.88320	-2.93371	3.96114
C	4.52914	-2.82019	2.12616
C	4.10853	-4.13817	1.83763
C	5.00580	-5.21571	1.94656
C	6.33936	-4.98923	2.33979
C	6.76797	-3.67674	2.61071
C	5.87154	-2.59726	2.49968
C	3.80219	-0.24652	3.43286

C	3.53537	3.40298	2.02928
C	4.66790	3.71467	1.25453
C	5.37789	4.91124	1.47709
C	4.96460	5.80499	2.48169
C	3.83563	5.49485	3.26703
C	3.12702	4.30158	3.04216
C	0.80231	2.36916	1.86599
C	0.42972	3.59969	1.28443
C	-0.90668	4.03618	1.32180
C	-1.89515	3.24796	1.94000
C	-1.53466	2.01043	2.50527
C	-0.19900	1.57090	2.45870
C	2.84103	0.95052	3.49808
C	5.25044	0.41586	0.62093
C	6.41670	0.54853	1.04345
C	7.75910	0.69521	1.53349
C	8.76974	-0.25199	1.20284
C	10.07883	-0.11151	1.69323
C	10.42001	0.97431	2.52546
C	9.43104	1.92173	2.86084
C	8.12047	1.78689	2.37327
C	1.29748	-0.12357	-0.53970
C	0.14848	-0.19089	-1.02155
C	-1.10935	-0.11411	-1.69117
C	-2.31106	0.55411	-1.22299
C	-3.31064	0.48863	-2.25829
C	-2.75646	-0.25129	-3.36837
C	-1.41408	-0.64097	-3.01220
Fe	-2.81218	-1.46468	-1.65835
C	-3.54510	-2.40923	0.08474
C	-2.38285	-3.11029	-0.39584
C	-2.66067	-3.57553	-1.73305
C	-3.99578	-3.16441	-2.07672
C	-4.56336	-2.45108	-0.94716
C	-5.91003	-1.87631	-0.91834
C	-6.54072	-1.35264	0.16853
Si	-8.27114	-0.61678	0.20701
Si	-9.61850	-1.80190	1.75033
Si	-11.78201	-0.87543	1.88176
Si	-11.63905	1.36781	2.58838
Si	-10.32737	2.58589	1.05637
Si	-11.33854	2.50367	-1.07032
Si	-8.17361	1.63664	0.92726
Si	-11.48786	0.26147	-1.78089
Si	-12.79476	-0.95683	-0.24429
Si	-9.32774	-0.67401	-1.90793
H	1.55503	-2.74329	-0.35529
H	0.29334	-4.85799	-0.72441
H	0.94958	-6.40115	-2.57717
H	2.89547	-5.81895	-4.04076
H	4.18197	-3.74314	-3.63304
H	5.29050	-4.06413	-0.85986
H	7.61981	-4.86923	-0.94469
H	9.42532	-3.42303	-1.90825
H	8.85224	-1.12495	-2.72322
H	6.53723	-0.30267	-2.60348
H	4.74401	-0.35526	-3.73571

H	3.36713	-1.40796	-4.09016
H	0.39268	1.94870	-2.68244
H	-1.13909	3.86406	-2.89655
H	-0.35405	6.18214	-2.36208
H	2.00282	6.53566	-1.58878
H	3.54894	4.61809	-1.39162
H	6.21792	1.75502	-1.09990
H	8.24009	2.76316	-2.12125
H	8.06237	4.06050	-4.25670
H	5.82474	4.34513	-5.34280
H	3.80288	3.36990	-4.30472
H	1.77753	0.24089	-3.16436
H	2.85475	1.12757	-4.27699
H	0.36950	-1.41331	1.29548
H	-1.64191	-2.36095	2.41494
H	-1.41190	-3.67763	4.52300
H	0.86058	-4.04232	5.51006
H	2.86412	-3.11021	4.39598
H	3.08111	-4.33319	1.54294
H	4.66134	-6.22437	1.73017
H	7.03215	-5.82263	2.43298
H	7.79739	-3.48423	2.90274
H	6.23152	-1.59264	2.69009
H	3.78214	-0.81391	4.37028
H	4.82277	0.08860	3.23490
H	5.01122	3.01486	0.50332
H	6.25234	5.13466	0.87035
H	5.51335	6.72821	2.65404
H	3.50780	6.17805	4.04720
H	2.24957	4.08309	3.64655
H	1.17343	4.22572	0.80238
H	-1.16956	4.98642	0.86362
H	-2.92731	3.58910	1.97664
H	-2.28772	1.38437	2.97885
H	0.03922	0.60021	2.88113
H	3.22819	1.71670	4.17755
H	1.86085	0.63725	3.87023
H	8.51124	-1.08772	0.55835
H	10.83439	-0.84818	1.42642
H	11.43398	1.08014	2.90459
H	9.68209	2.76382	3.50289
H	7.36094	2.51966	2.63518
H	-2.40129	1.05012	-0.26735
H	-4.30704	0.90499	-2.20411
H	-3.25746	-0.47461	-4.30014
H	-0.72963	-1.21795	-3.61846
H	-3.64543	-1.92999	1.04857
H	-1.45394	-3.23860	0.13863
H	-1.97801	-4.12091	-2.36882
H	-4.50547	-3.35980	-3.01088
H	-6.43254	-1.90221	-1.87765
H	-6.00255	-1.35492	1.12028
H	-8.98101	-1.76488	3.09538
H	-9.71498	-3.22671	1.33298
H	-12.60351	-1.65173	2.85214
H	-11.02646	1.43380	3.94241
H	-13.00036	1.96173	2.67235

H	-10.22566	4.00373	1.50229
H	-10.53397	3.28937	-2.04414
H	-12.69870	3.10305	-1.01072
H	-7.34133	2.42531	-0.02204
H	-7.51887	1.70493	2.26313
H	-12.12225	0.20799	-3.12769
H	-14.16211	-0.37457	-0.17831
H	-12.91863	-2.36925	-0.69397
H	-9.42271	-2.07897	-2.39004
H	-8.51757	0.08575	-2.89940

Figure S24. HOMO of complex **Si-4** (-4.44 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.



Geometry Optimization of Complex Si-4$^+$

Input file:

```
%chk=F4SiH1SP

#B3LYP/LanL2DZ opt

F4SiH1SP

  1  2
```

Cartesian Coordinates for the Optimized Geometry of Complex **Si-4**$^+$ (-3148.2872186 Hartrees)

Ru	3.28983	0.12726	0.03531

P	3.91215	-1.52178	-1.72824
P	3.43923	1.72860	-1.91092
C	2.83478	-3.04461	-2.03179
C	1.77843	-3.38220	-1.16556
C	1.00222	-4.53393	-1.40314
C	1.26989	-5.35401	-2.51386
C	2.31965	-5.01555	-3.39152
C	3.09846	-3.87097	-3.14942
C	5.64962	-2.25900	-1.79683
C	5.88585	-3.58582	-1.38067
C	7.18116	-4.13137	-1.43981
C	8.25661	-3.35814	-1.91449
C	8.02999	-2.02590	-2.30986
C	6.73745	-1.47641	-2.24052
C	3.80354	-0.62156	-3.42531
C	2.29487	3.21977	-2.03438
C	0.96840	3.09355	-2.49784
C	0.14150	4.22745	-2.60547
C	0.62584	5.49737	-2.24178
C	1.94547	5.62707	-1.76590
C	2.77409	4.49589	-1.66098
C	5.04861	2.45226	-2.60452
C	6.29800	2.23107	-1.99303
C	7.47267	2.76222	-2.56412
C	7.41003	3.51215	-3.75164
C	6.16199	3.73415	-4.36888
C	4.98969	3.21031	-3.79881
C	2.90902	0.62501	-3.36874
P	3.28674	-1.44006	1.99146
P	2.69107	1.77599	1.81517
C	1.70602	-2.16720	2.74384
C	0.43335	-1.86650	2.22215
C	-0.72726	-2.35441	2.85743
C	-0.62749	-3.14579	4.01478
C	0.64472	-3.45252	4.53852
C	1.80259	-2.96534	3.90898
C	4.45665	-2.91177	2.07480
C	3.98054	-4.20450	1.75984
C	4.83359	-5.31876	1.84758
C	6.17512	-5.15378	2.24358
C	6.65748	-3.86619	2.54147
C	5.80593	-2.74926	2.45420
C	3.84193	-0.32207	3.42843
C	3.68981	3.36172	2.06528
C	4.83245	3.63859	1.29209
C	5.58105	4.80984	1.52167
C	5.19574	5.71128	2.53040
C	4.05570	5.43562	3.31230
C	3.30752	4.26822	3.08169
C	0.91701	2.42540	1.91846
C	0.58666	3.64492	1.28828
C	-0.72386	4.15088	1.34921
C	-1.72689	3.44559	2.04036
C	-1.40951	2.21919	2.65365
C	-0.09994	1.70754	2.58339
C	2.92720	0.90868	3.51828
C	5.25998	0.31492	0.59925

C	6.42784	0.39294	1.03047
C	7.76879	0.49482	1.53488
C	8.77108	-0.43299	1.13705
C	10.07726	-0.33524	1.64343
C	10.41606	0.68930	2.55081
C	9.43290	1.61728	2.95114
C	8.12364	1.52238	2.45294
C	1.36764	-0.02680	-0.52112
C	0.18984	-0.01220	-0.97220
C	-1.08325	0.14821	-1.53849
C	-2.27062	0.70395	-0.89202
C	-3.33244	0.75574	-1.85317
C	-2.85832	0.16402	-3.08330
C	-1.50057	-0.25550	-2.88248
Fe	-2.78864	-1.27195	-1.52694
C	-3.65827	-2.41427	0.07523
C	-2.47702	-3.07999	-0.39940
C	-2.66502	-3.39046	-1.79258
C	-3.97980	-2.93288	-2.16876
C	-4.61794	-2.34856	-1.01116
C	-5.97040	-1.77972	-0.99566
C	-6.64816	-1.36617	0.10858
Si	-8.39186	-0.64187	0.15213
Si	-9.77500	-1.96936	1.53843
Si	-11.93909	-1.04512	1.67279
Si	-11.80921	1.11742	2.59909
Si	-10.45621	2.47207	1.22579
Si	-11.38004	2.59513	-0.93862
Si	-8.29988	1.53157	1.08434
Si	-11.52029	0.42944	-1.85771
Si	-12.87381	-0.92835	-0.48728
Si	-9.35954	-0.50107	-1.99939
H	1.55140	-2.74689	-0.31744
H	0.20093	-4.79509	-0.71599
H	0.67513	-6.24642	-2.69296
H	2.53786	-5.64434	-4.25089
H	3.92331	-3.64296	-3.82067
H	5.06998	-4.20322	-1.01962
H	7.34392	-5.15680	-1.11840
H	9.25474	-3.78495	-1.97398
H	8.85351	-1.41381	-2.66895
H	6.59841	-0.43924	-2.52877
H	4.81939	-0.35182	-3.72877
H	3.41682	-1.33733	-4.15736
H	0.56756	2.12685	-2.78102
H	-0.87525	4.11453	-2.97294
H	-0.01068	6.37381	-2.33493
H	2.33309	6.60323	-1.48585
H	3.79351	4.61843	-1.30759
H	6.36190	1.64769	-1.08216
H	8.42843	2.58673	-2.07659
H	8.31645	3.92125	-4.19083
H	6.10163	4.31526	-5.28557
H	4.03473	3.41097	-4.27859
H	1.86459	0.34648	-3.20976
H	2.98685	1.19961	-4.29831
H	0.34215	-1.24988	1.33432

H	-1.70423	-2.10079	2.45409
H	-1.52359	-3.52003	4.50333
H	0.73460	-4.06558	5.43151
H	2.77546	-3.21937	4.32211
H	2.94513	-4.35421	1.46723
H	4.44874	-6.30882	1.61603
H	6.83224	-6.01630	2.32246
H	7.69203	-3.72431	2.84277
H	6.20599	-1.76710	2.67910
H	3.80661	-0.89930	4.35908
H	4.87370	-0.02561	3.23084
H	5.15461	2.93717	0.53316
H	6.46250	5.00893	0.91711
H	5.77405	6.61452	2.70824
H	3.75008	6.12555	4.09480
H	2.42236	4.07862	3.68421
H	1.34498	4.21390	0.76046
H	-0.95406	5.09458	0.86184
H	-2.73561	3.84633	2.10349
H	-2.17255	1.66422	3.19466
H	0.10317	0.75231	3.05628
H	3.35172	1.64978	4.20285
H	1.94301	0.62632	3.90254
H	8.51046	-1.22123	0.43652
H	10.83162	-1.05390	1.33170
H	11.42845	0.76329	2.93989
H	9.68795	2.40965	3.65072
H	7.36687	2.23885	2.76268
H	-2.29028	1.09600	0.11432
H	-4.32513	1.14705	-1.68010
H	-3.42942	0.04883	-3.99390
H	-0.86023	-0.73213	-3.61143
H	-3.82326	-2.05477	1.08103
H	-1.58980	-3.28281	0.18273
H	-1.95540	-3.89060	-2.43585
H	-4.43221	-3.02972	-3.14681
H	-6.44963	-1.71855	-1.97454
H	-6.15011	-1.46166	1.07814
H	-9.16638	-2.04747	2.89461
H	-9.83887	-3.34789	0.98426
H	-12.78478	-1.91188	2.53817
H	-11.22448	1.04780	3.96423
H	-13.16909	1.70797	2.70142
H	-10.35156	3.83948	1.80535
H	-10.52421	3.45307	-1.80059
H	-12.73533	3.20166	-0.87557
H	-7.42277	2.38666	0.23647
H	-7.67657	1.45850	2.43513
H	-12.09797	0.50226	-3.22762
H	-14.24132	-0.35124	-0.41359
H	-12.97000	-2.29226	-1.07030
H	-9.42074	-1.85804	-2.60750
H	-8.49672	0.34047	-2.87486

Figure S25. SOMO of complex **Si-4**$^{+}$ (-7.18 eV) shown with a cutoff of 0.05 [e/Bohr^{3}]$^{1/2}$.

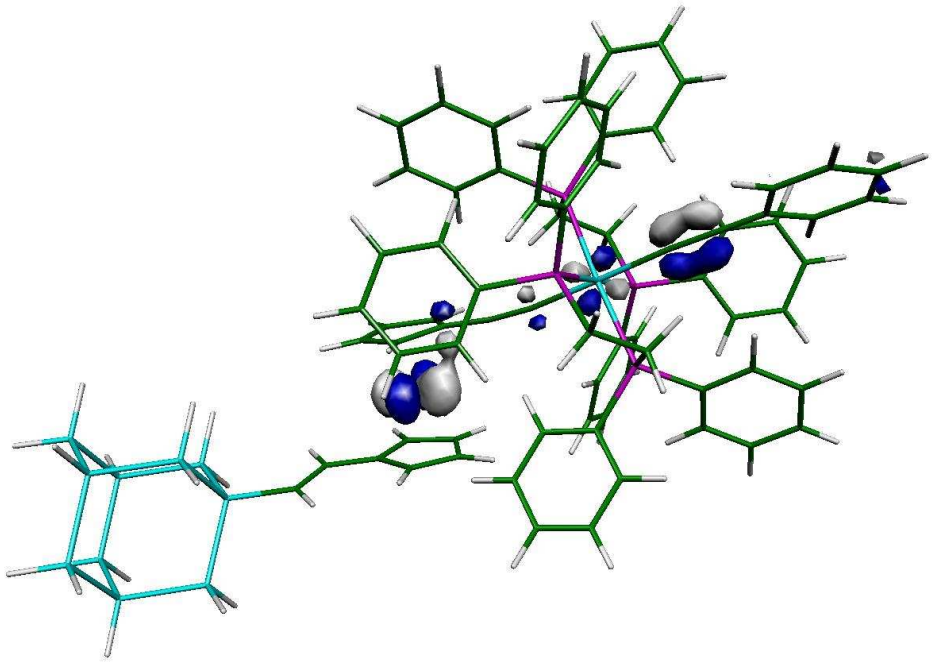
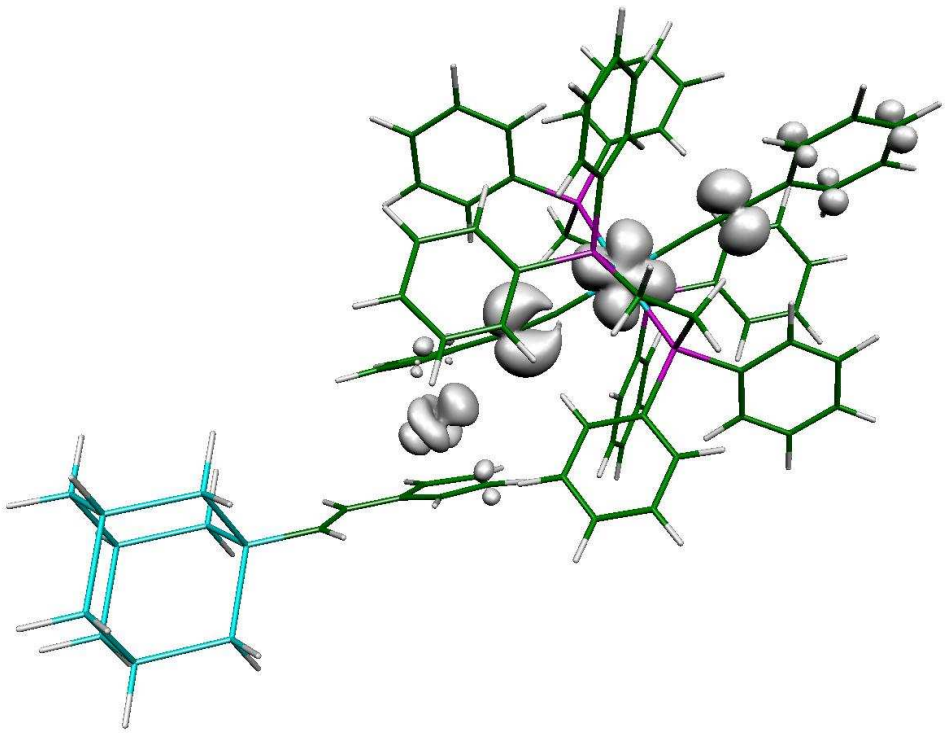


Figure S26. Spin density for complex **Si-4**$^{+}$ shown with a cut-off of 0.002 e/Bohr^{3}.



Geometry Optimization of Complex Si-4^{2+}

Input file:

```
%chk= F4SiH2

#B3LYP/LanL2DZ opt

F4SiH2

  2  3
```

Cartesian Coordinates for the Optimized Geometry of Complex **Si-4**$^{2+}$ (-3148.0184213 Hartrees)

Ru	4.37366	0.21814	0.03529
P	4.78161	-1.66985	-1.56179
P	4.46725	1.55560	-2.11944
C	3.62790	-3.16461	-1.56296
C	2.60696	-3.30515	-0.60538
C	1.77898	-4.44531	-0.60929
C	1.95587	-5.44758	-1.58090
C	2.96720	-5.30410	-2.55260
C	3.80104	-4.17248	-2.54040
C	6.48020	-2.48925	-1.65248
C	6.71312	-3.70255	-0.96993
C	7.96834	-4.33265	-1.04450
C	9.00775	-3.75909	-1.80059
C	8.78777	-2.53711	-2.46432
C	7.53596	-1.89980	-2.38163
C	4.55676	-0.98494	-3.34448
C	3.44989	3.11921	-2.35580
C	2.10121	3.06799	-2.76518
C	1.37693	4.25626	-2.97535
C	1.98917	5.50648	-2.77106
C	3.33263	5.56264	-2.35142
C	4.05856	4.37684	-2.14299
C	6.08763	2.03505	-2.97431
C	7.34971	1.78224	-2.40535
C	8.52546	2.13847	-3.09655
C	8.44825	2.74255	-4.36382
C	7.18621	2.99351	-4.94003
C	6.01305	2.64607	-4.24960
C	3.75376	0.32321	-3.38091
P	4.27501	-1.12723	2.18641
P	3.98056	2.11697	1.63647
C	2.66772	-1.63001	3.05139
C	1.40346	-1.30297	2.52422
C	0.23230	-1.63334	3.23648
C	0.31310	-2.29071	4.47696
C	1.57669	-2.62245	5.00590
C	2.74604	-2.29405	4.29903
C	5.33855	-2.66280	2.40792
C	4.76415	-3.94457	2.25284
C	5.54099	-5.10035	2.44766
C	6.90166	-4.98925	2.79420
C	7.48024	-3.71471	2.93762
C	6.70553	-2.55654	2.74181

C	4.97675	0.10761	3.45412
C	5.14741	3.60086	1.66991
C	6.22115	3.71958	0.76789
C	7.09042	4.82610	0.83721
C	6.89379	5.82132	1.81168
C	5.82024	5.70722	2.71811
C	4.95146	4.60459	2.64773
C	2.28240	2.94246	1.70900
C	2.05904	4.14193	0.99968
C	0.80700	4.78063	1.05119
C	-0.23925	4.23295	1.81656
C	-0.02761	3.02827	2.51370
C	1.22021	2.38022	2.45028
C	4.17892	1.41762	3.41663
C	6.31530	0.29379	0.47034
C	7.52339	0.32133	0.82831
C	8.88288	0.38044	1.23684
C	9.84319	-0.54058	0.71694
C	11.17886	-0.47907	1.13341
C	11.58859	0.49979	2.06619
C	10.65124	1.42043	2.58624
C	9.31213	1.36314	2.18203
C	2.36220	0.16839	-0.41624
C	1.16648	0.23386	-0.78369
C	-0.15464	0.46125	-1.21931
C	-1.28383	0.89218	-0.41247
C	-2.42036	1.09619	-1.26922
C	-2.04014	0.71676	-2.61044
C	-0.67100	0.27208	-2.56827
Fe	-1.95616	-0.98287	-1.34434
C	-3.24517	-2.24176	-0.11657
C	-1.88696	-2.72607	-0.11352
C	-1.53650	-3.06990	-1.47036
C	-2.68518	-2.80090	-2.29763
C	-3.77900	-2.35288	-1.46044
C	-5.11071	-2.00996	-1.94580
C	-6.18392	-1.69892	-1.16096
Si	-7.93560	-1.29570	-1.76019
Si	-9.45752	-2.84220	-0.80947
Si	-11.65065	-2.30395	-1.48899
Si	-12.19267	-0.14425	-0.71834
Si	-10.69293	1.41420	-1.65394
Si	-10.80736	1.35716	-4.00728
Si	-8.49911	0.86986	-0.98194
Si	-10.29121	-0.81250	-4.76990
Si	-11.77912	-2.38667	-3.84063
Si	-8.09154	-1.34946	-4.11568
H	2.45203	-2.53199	0.13798
H	1.01552	-4.55941	0.15733
H	1.32545	-6.33324	-1.57771
H	3.11612	-6.07529	-3.30354
H	4.59833	-4.09657	-3.27608
H	5.92429	-4.17133	-0.39084
H	8.12691	-5.27103	-0.52013
H	9.97052	-4.25781	-1.87559
H	9.58162	-2.08311	-3.05188
H	7.40772	-0.95188	-2.89472

H	5.54885	-0.83386	-3.77789
H	4.05365	-1.75852	-3.93305
H	1.60970	2.11654	-2.93581
H	0.34235	4.20449	-3.30478
H	1.43311	6.42350	-2.94737
H	3.81822	6.52281	-2.19913
H	5.09929	4.44135	-1.84026
H	7.42650	1.30665	-1.43535
H	9.49366	1.94359	-2.64253
H	9.35481	3.01802	-4.89600
H	7.11627	3.46283	-5.91761
H	5.04967	2.87049	-4.70095
H	2.70948	0.14558	-3.11528
H	3.79803	0.77337	-4.37861
H	1.32939	-0.78964	1.57221
H	-0.73964	-1.35934	2.83079
H	-0.59005	-2.54061	5.02753
H	1.65134	-3.13186	5.96271
H	3.71037	-2.56873	4.71865
H	3.71252	-4.05208	2.00458
H	5.08253	-6.07990	2.34040
H	7.49847	-5.88237	2.95940
H	8.52848	-3.61760	3.20684
H	7.17850	-1.58779	2.86068
H	4.92544	-0.34663	4.44972
H	6.02491	0.28282	3.20239
H	6.39527	2.95316	0.02289
H	7.91673	4.90534	0.13533
H	7.56418	6.67502	1.86556
H	5.65808	6.47359	3.47130
H	4.11712	4.54430	3.34282
H	2.85641	4.59533	0.42040
H	0.65869	5.70898	0.50634
H	-1.19731	4.74259	1.87931
H	-0.82053	2.60476	3.12642
H	1.34401	1.45012	2.99602
H	4.68142	2.18511	4.01339
H	3.18288	1.26912	3.84178
H	9.51992	-1.29164	0.00244
H	11.90386	-1.18534	0.73840
H	12.62674	0.54526	2.38447
H	10.97160	2.17316	3.30102
H	8.58757	2.07296	2.57222
H	-1.22911	1.11965	0.64229
H	-3.38158	1.48731	-0.96592
H	-2.66249	0.77687	-3.49236
H	-0.08846	-0.07263	-3.41170
H	-3.79588	-1.91166	0.75351
H	-1.25265	-2.82706	0.75576
H	-0.59280	-3.47794	-1.80304
H	-2.75190	-2.97075	-3.36435
H	-5.23189	-2.05176	-3.02842
H	-6.03744	-1.69101	-0.07575
H	-9.32242	-2.78021	0.67060
H	-9.07688	-4.20777	-1.25607
H	-12.57682	-3.30436	-0.89492
H	-12.09597	-0.09867	0.76327

H	-13.57924	0.19972	-1.12184
H	-10.99676	2.78484	-1.16199
H	-9.83887	2.33003	-4.57709
H	-12.17465	1.73014	-4.44933
H	-7.51215	1.83803	-1.53653
H	-8.36329	0.89181	0.50028
H	-10.35492	-0.85837	-6.25515
H	-13.16314	-2.07210	-4.27597
H	-11.42231	-3.74797	-4.31614
H	-7.70046	-2.70223	-4.59749
H	-7.11317	-0.37785	-4.68103

Figure S27. SOMO of complex **Si-4**$^{2+}$ (-9.63 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

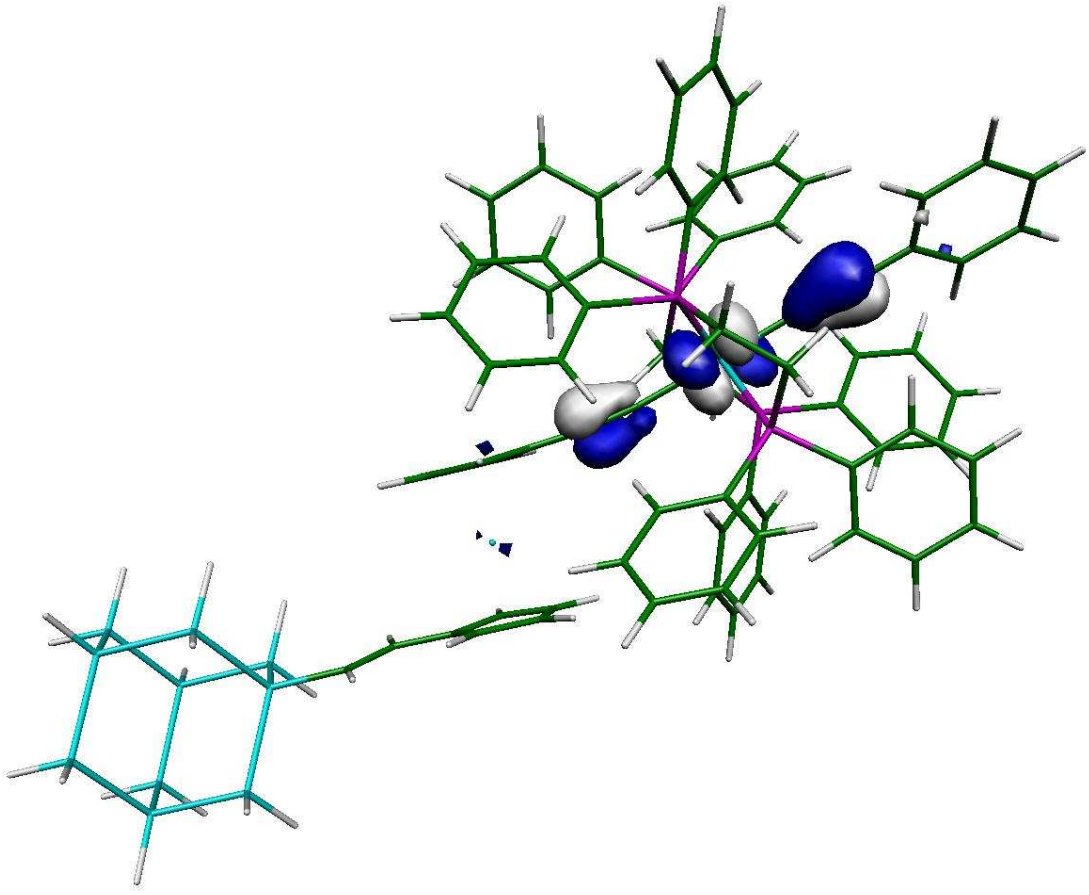


Figure S28. SOMO-1 of complex **Si-4**$^{2+}$ (-9.75 eV) shown with a cutoff of 0.05 [e/Bohr^3]$^{1/2}$.

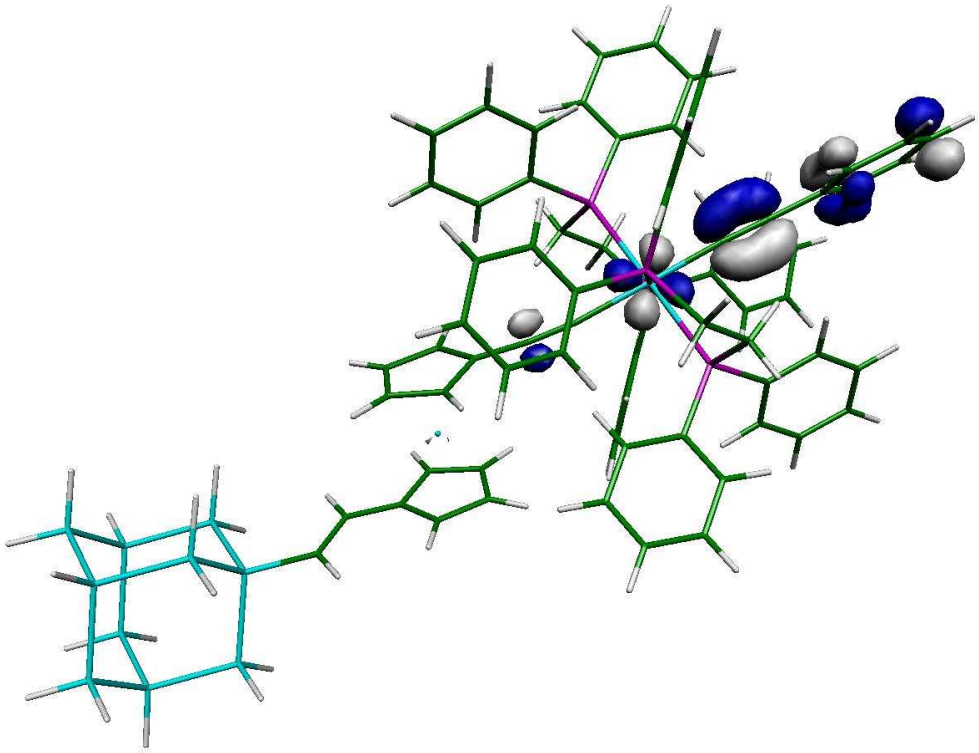
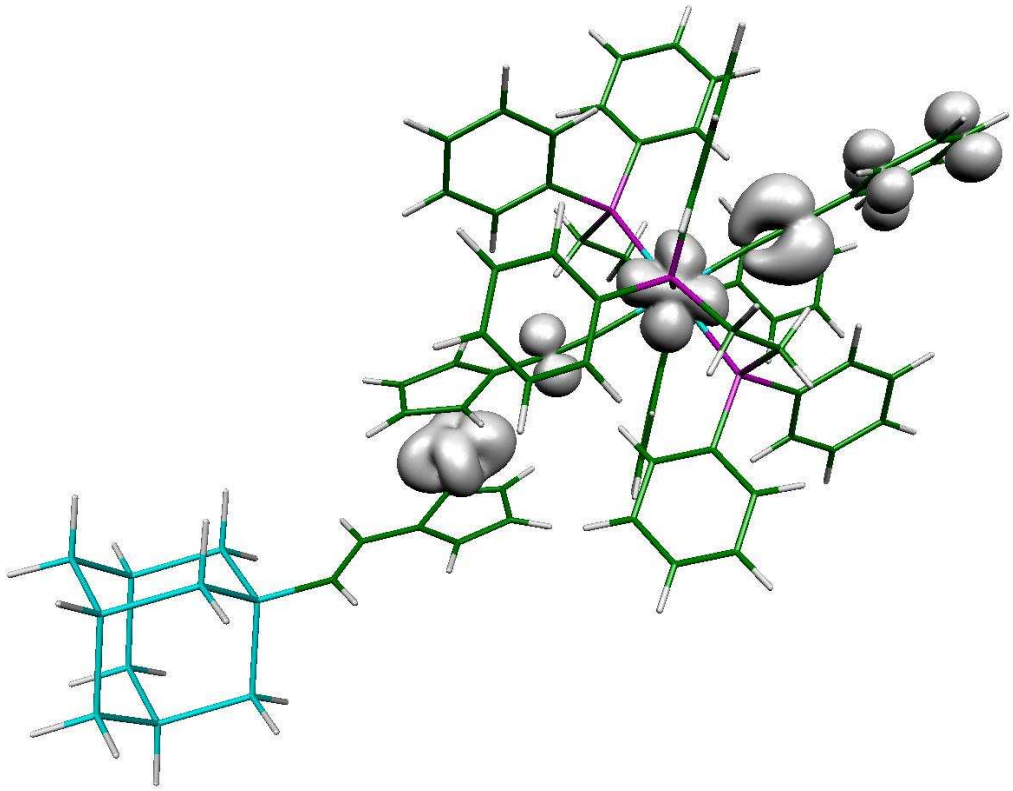


Figure S29. Spin density for complex **Si-4**$^{2+}$ shown with a cut-off of 0.002 e/Bohr^3.



10. References for Gaussian 03 and Molekel 4.3 softwares

References for the Gaussian 03 software

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References for the Molekel 4.3 software used to generate the figures

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