

## Supporting Information

### Ferrocene Analogues of Sandwich $M(\text{CrB}_6\text{H}_6)_2$ : A Theoretical Investigation

**by**

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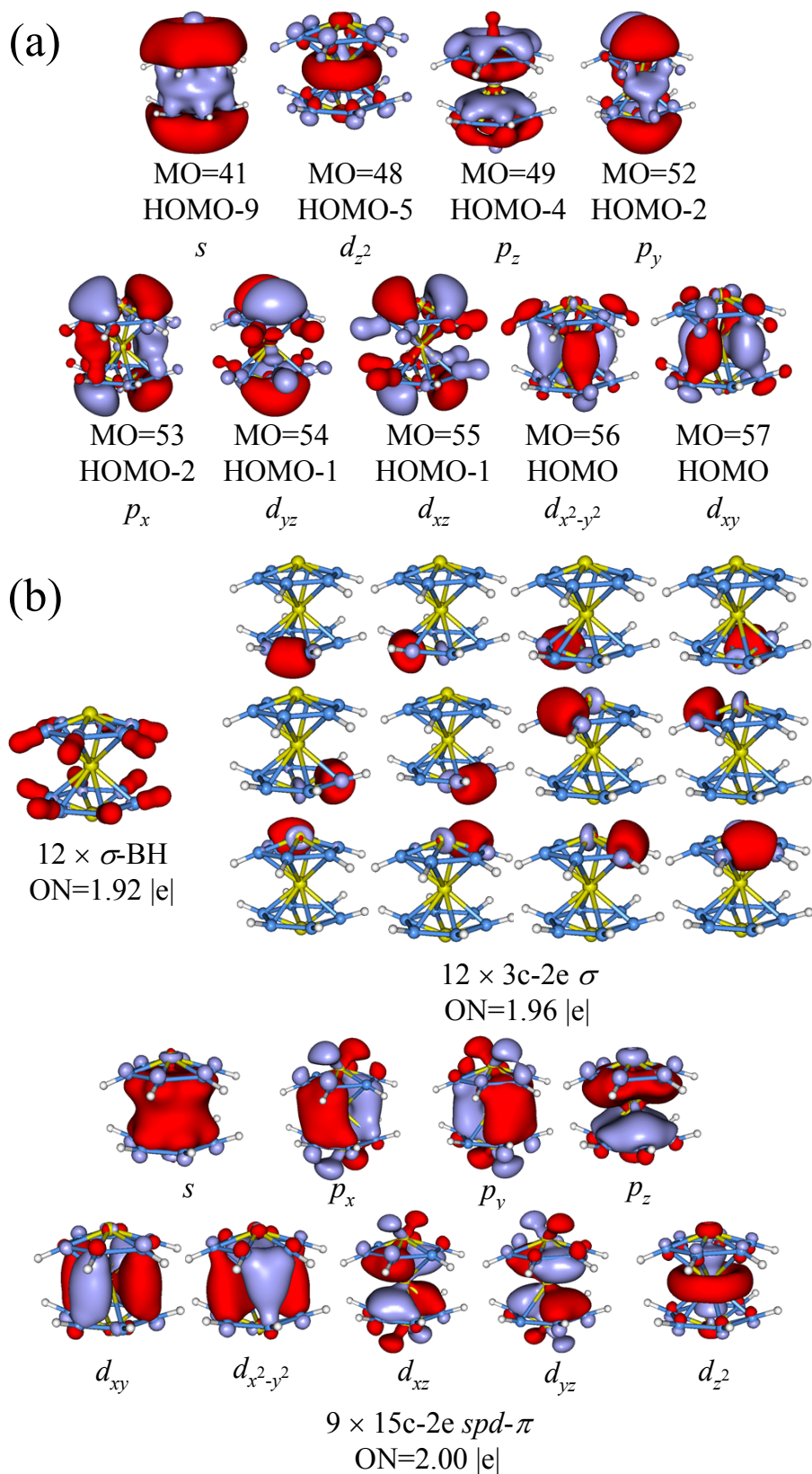
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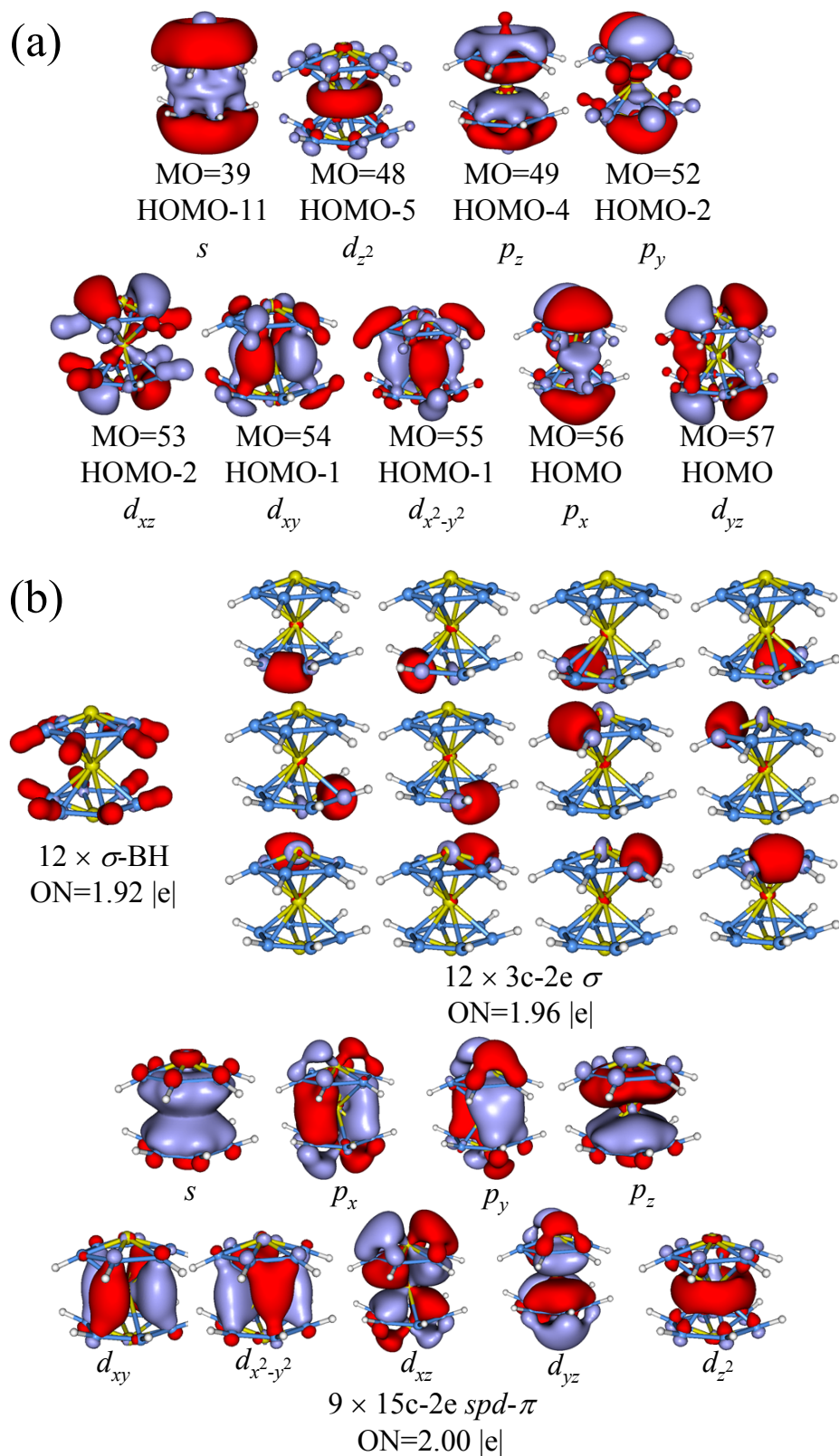
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**Figure S1.** (a) Partial canonical molecular orbitals and (b) AdNDP localized bonding patterns of  $[\text{Mn}(\text{CrB}_6\text{H}_6)_2]^+$ .



**Figure S2.** (a) Partial canonical molecular orbitals and (b) AdNDP localized bonding patterns of  $[\text{Fe}(\text{CrB}_6\text{H}_6)_2]^{2+}$ .

Coordinates of  $M(\text{CrB}_6\text{H}_6)_2$  ( $M = \text{Cr}, \text{Mn}^+, \text{Fe}^{2+}$ ) (in angstrom):

Cr(CrB<sub>6</sub>H<sub>6</sub>)<sub>2</sub>

Cr	0.000000	0.000000	2.153838
B	0.000000	1.834798	1.524821
B	-1.588982	0.917399	1.524821
B	-1.588982	-0.917399	1.524821
B	0.000000	-1.834798	1.524821
B	1.588982	-0.917399	1.524821
B	1.588982	0.917399	1.524821
H	0.000000	2.966923	1.177759
H	-2.569431	1.483461	1.177759
H	-2.569431	-1.483461	1.177759
H	0.000000	-2.966923	1.177759
H	2.569431	-1.483461	1.177759
H	2.569431	1.483461	1.177759
Cr	0.000000	0.000000	0.000000
Cr	0.000000	0.000000	-2.153838
B	-0.917399	1.588982	-1.524821
B	-1.834798	0.000000	-1.524821
B	-0.917399	-1.588982	-1.524821
B	0.917399	-1.588982	-1.524821
B	1.834798	0.000000	-1.524821
B	0.917399	1.588982	-1.524821
H	-1.483461	2.569431	-1.177759
H	-2.966923	0.000000	-1.177759
H	-1.483461	-2.569431	-1.177759
H	1.483461	-2.569431	-1.177759
H	2.966923	0.000000	-1.177759
H	1.483461	2.569431	-1.177759

[Mn(CrB<sub>6</sub>H<sub>6</sub>)<sub>2</sub>]<sup>+</sup>

Cr	0.000000	0.000000	2.139356
B	0.000000	1.840842	1.540099
B	-1.594216	0.920421	1.540099
B	-1.594216	-0.920421	1.540099
B	0.000000	-1.840842	1.540099
B	1.594216	-0.920421	1.540099
B	1.594216	0.920421	1.540099
H	0.000000	2.955466	1.146528
H	-2.559508	1.477733	1.146528
H	-2.559508	-1.477733	1.146528
H	0.000000	-2.955466	1.146528
H	2.559508	-1.477733	1.146528
H	2.559508	1.477733	1.146528

Mn	0.000000	0.000000	0.000000
Cr	0.000000	0.000000	-2.139356
B	-0.920421	1.594216	-1.540099
B	-1.840842	0.000000	-1.540099
B	-0.920421	-1.594216	-1.540099
B	0.920421	-1.594216	-1.540099
B	1.840842	0.000000	-1.540099
B	0.920421	1.594216	-1.540099
H	-1.477733	2.559508	-1.146528
H	-2.955466	0.000000	-1.146528
H	-1.477733	-2.559508	-1.146528
H	1.477733	-2.559508	-1.146528
H	2.955466	0.000000	-1.146528
H	1.477733	2.559508	-1.146528
<u>[Fe(CrB<sub>6</sub>H<sub>6</sub>)<sub>2</sub>]<sup>2+</sup></u>			
Cr	0.000000	0.000000	2.159098
B	0.000000	1.850757	1.573630
B	-1.602802	0.925378	1.573630
B	-1.602802	-0.925378	1.573630
B	0.000000	-1.850757	1.573630
B	1.602802	-0.925378	1.573630
B	1.602802	0.925378	1.573630
H	0.000000	2.951246	1.142094
H	-2.555854	1.475623	1.142094
H	-2.555854	-1.475623	1.142094
H	0.000000	-2.951246	1.142094
H	2.555854	-1.475623	1.142094
H	2.555854	1.475623	1.142094
Fe	0.000000	0.000000	0.000000
Cr	0.000000	0.000000	-2.159098
B	-0.925378	1.602802	-1.573630
B	-1.850757	0.000000	-1.573630
B	-0.925378	-1.602802	-1.573630
B	0.925378	-1.602802	-1.573630
B	1.850757	0.000000	-1.573630
B	0.925378	1.602802	-1.573630
H	-1.475623	2.555854	-1.142094
H	-2.951246	0.000000	-1.142094
H	-1.475623	-2.555854	-1.142094
H	1.475623	-2.555854	-1.142094
H	2.951246	0.000000	-1.142094
H	1.475623	2.555854	-1.142094