

Supplementary Materials

Electronic and Structural Properties of the Double Cubane Iron-Sulfur Cluster

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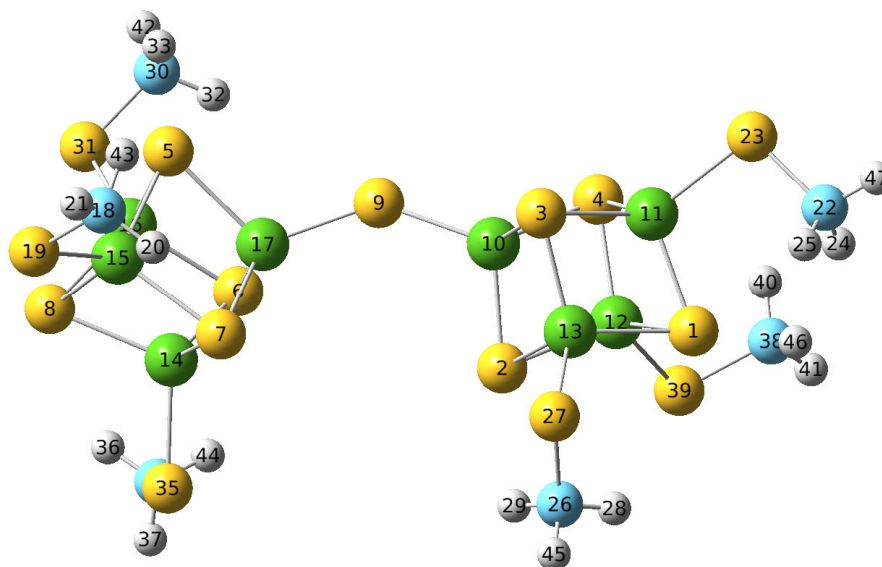


Figure S1. Atoms considered in the QM geometry optimizations of the DCC active site are shown. Fe atoms are colored in green, sulfur atoms in yellow, carbon atoms in blue, and hydrogen atoms in grey.

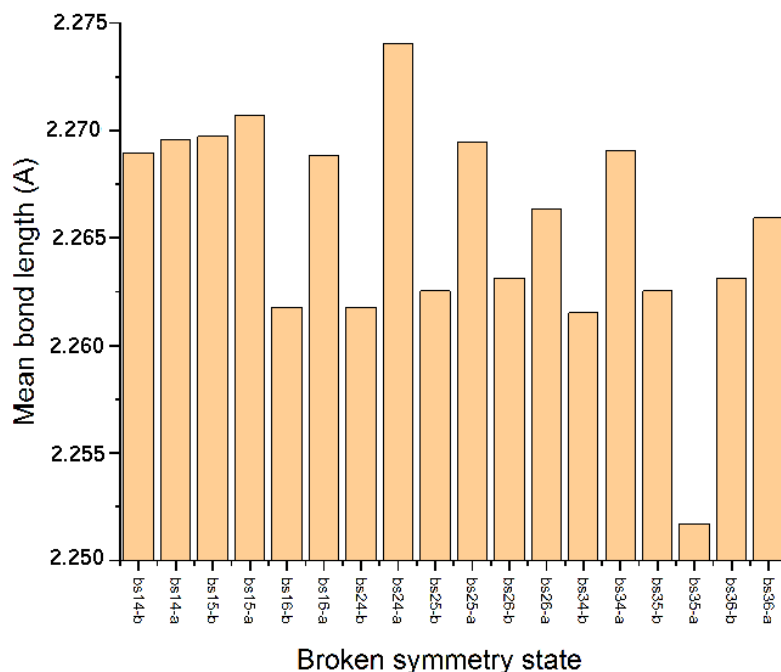


Figure S2. The QM/MM geometry optimized average cluster bond lengths for each of the nine broken symmetry states. Plot drawn with Origin and TGIF.

Table S1. QM energies.

BS state	Energy (Hartree)	Energy (eV)
HS1 aaaa-aaaa	-16561.62453159	-613.39350117
HS2 aaaa-bbbb	-16561.75576231	-613.39836157
BS14 bbba-abba	-16561.77764837	-613.39917216
BS15 bbba-baba	-16561.77555852	-613.39909476
BS16 bbba-bbaa	-16561.77888329	-613.39921790
BS24 baba-abba	-16561.77700987	-613.39914851
BS25 baba-baba	-16561.77534911	-613.39908700
BS26 baba-bbaa	-16561.778856610	-613.39921691
BS34 baab-abba	-16561.77711173	-613.39915229
BS35 baab-baba	-16561.77502449	-613.39907498
BS36 baab-bbaa	-16561.77822721	-613.39919360
BS52 baba-abab	-16561.78514901	-613.39944996
BS17 bbba-aaaa	-16561.71733787	-613.39693844
BS18 aabb-aaaa	-16561.69859719	-613.39624434
BS27 baba-aaaa	-16561.71798339	-613.39696235
BS28 abab-aaaa	-16561.69917888	-613.39626588
BS37 abba-aaaa	-16561.70109859	-613.39633698
BS38 baab-aaaa	-16561.71991102	-613.39703374
BS44 aaaa-abba	-16561.71518017	-613.39685852
BS45 aaaa-abab	-16561.69918861	-613.39626624

BS46 aaaa-aabb	−16561.70071008	−613.3963226
BS54 aaaa-baab	−16561.72097472	−613.39707314
BS55 aaaa-baba	−16561.71781437	−613.39695609
BS56 aaaa-bbaa	−16561.71938602	−613.39701430

Table S2. Fe–S bond lengths of A-subcluster of BS25.

BS25 A cluster	distance (Å)	type
Fe8–S9	2.17	-
Fe8–S5	2.31	l
Fe8–S6	2.24	s
Fe8–S7	2.28	l
Fe7–S5	2.19	s
Fe7–S6	2.30	l
Fe7–S8	2.27	l
Fe6–S5	2.29	l
Fe6–S7	2.30	l
Fe6–S8	2.20	s
Fe5–S6	2.35	l
Fe5–S7	2.19	s
Fe5–S8	2.30	l