

Supporting Information

**Understanding the stability, bonding nature and chemical reactivity of 3d-substituted heterofullerenes C<sub>58</sub>TM (TM=Sc-Zn) from DFT study**

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Table S1. The total energies of different spin multiplicities for studied [6:6] isomers.

Species	Spin multiplicity	Total energy
C <sub>58</sub> Sc	2	-2256.335449
	4	-2256.290212
C <sub>58</sub> Ti	1	-2267.853345
	3	-2267.827127
C <sub>58</sub> V	2	-2281.128903
	4	-2281.106386
C <sub>58</sub> Cr	1	-2296.285490
	3	-2296.350446
	5	-2296.337705
C <sub>58</sub> Mn	2	-2313.638802
	4	-2313.685258
	6	-2313.676446
C <sub>58</sub> Fe	1	-2333.057868
	3	-2333.135548
	5	-2333.149262
	7	-2333.084332
C <sub>58</sub> Co	2	-2354.979916
	4	-2354.972662
C <sub>58</sub> Ni	1	-2379.293412
	3	-2379.283189
C <sub>58</sub> Cu	2	-2406.244143
	4	-2406.186901
C <sub>58</sub> Zn	1	-2435.609229
	3	-2435.580858

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