SUPPLEMENTARY INFORMATION (SI)

Nitrogen reduction reaction on single cluster catalysts of defective PC_6-trimeric or tetrameric transition metal

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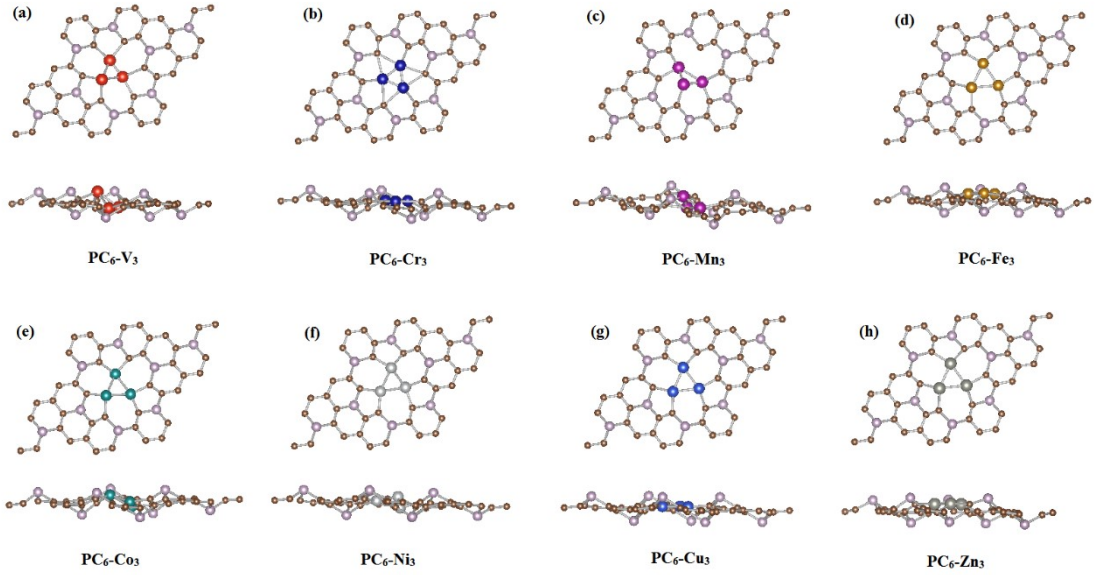

Fig. S1 Optimized geometric configurations of PC_6-TM_3.

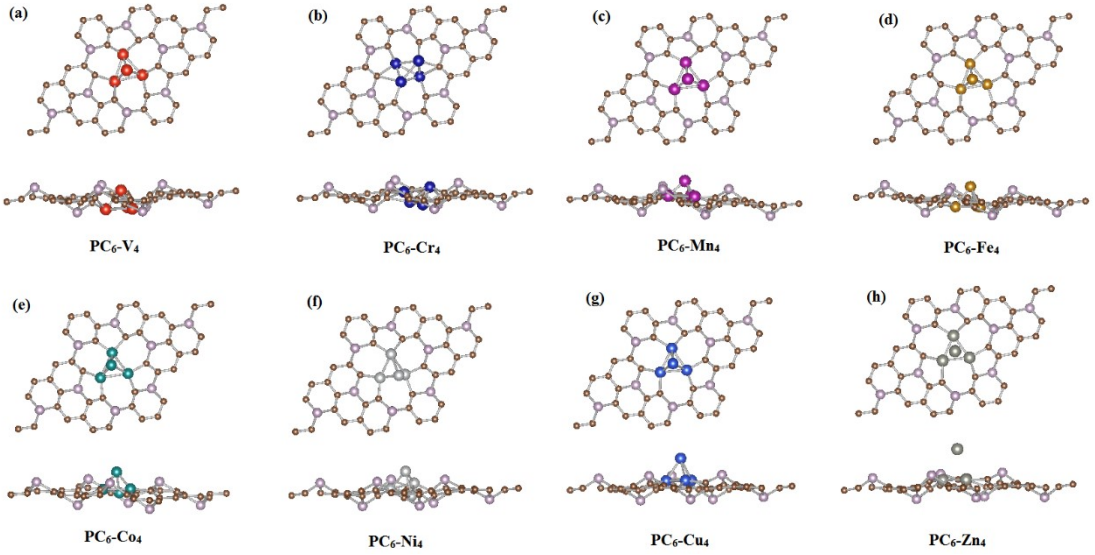

Fig. S2 Optimized geometric configurations of PC_6-TM_4.

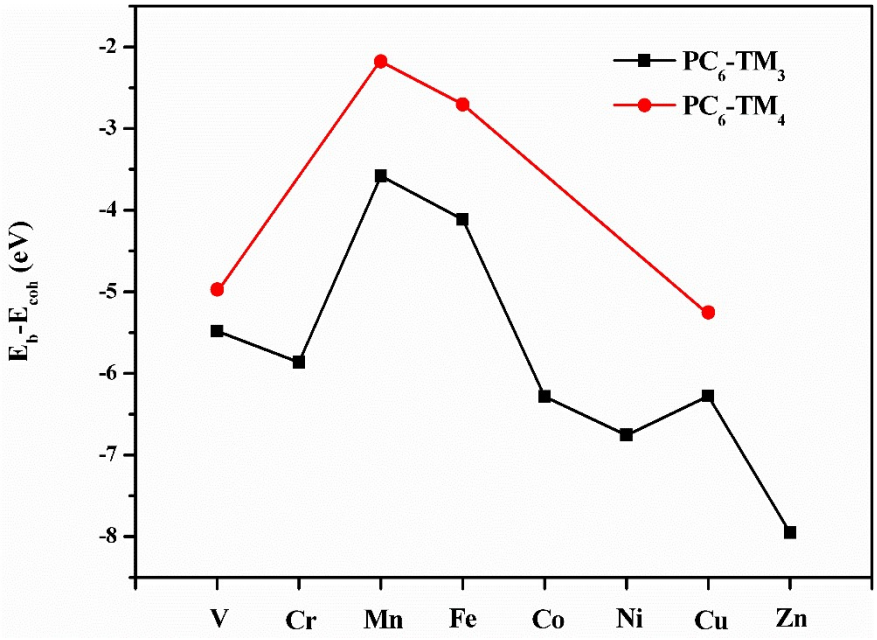

Fig. S3 The calculated E_b-E_{coh} values of PC_6-TM_3 and PC_6-TM_4.

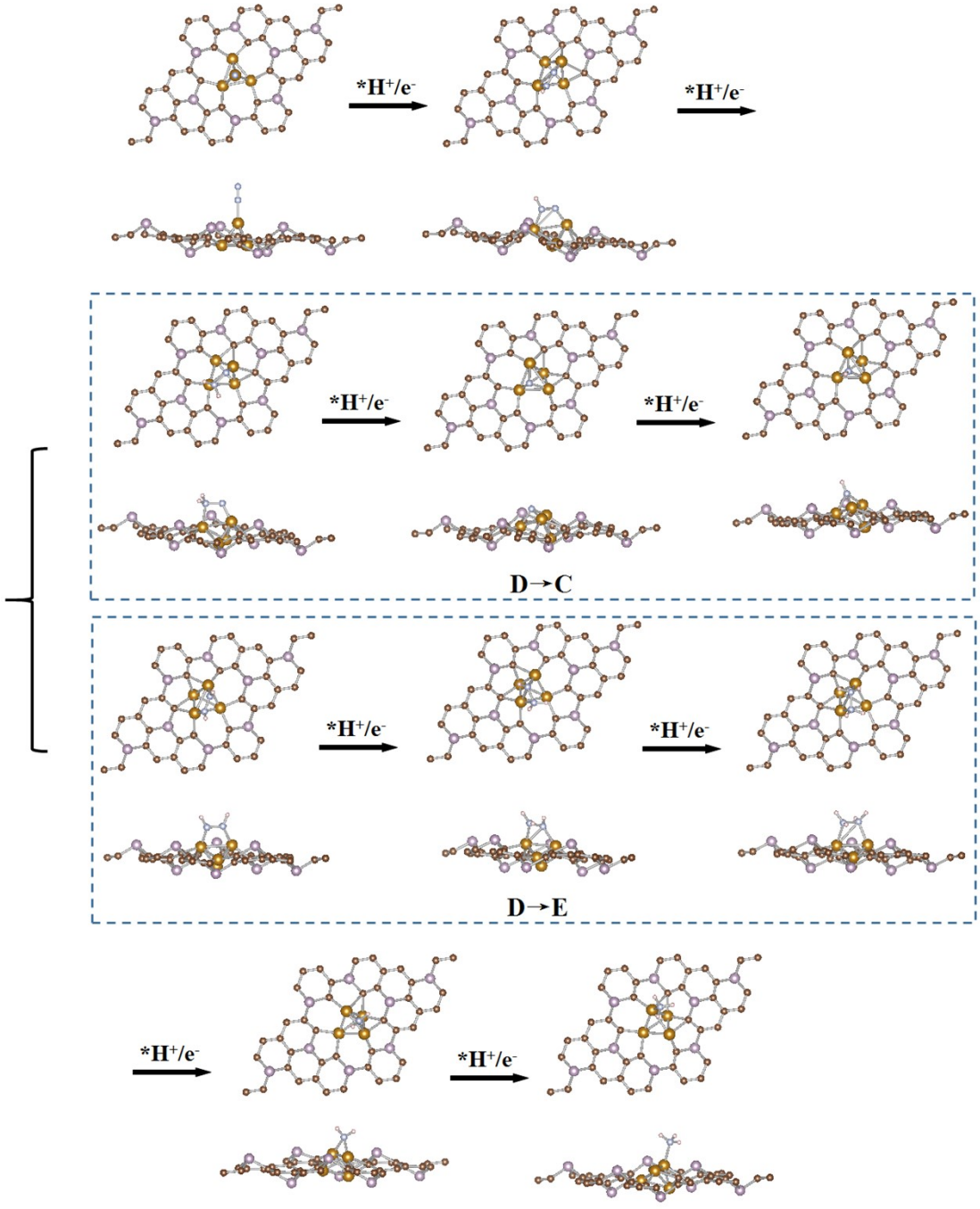

Fig. S4 The optimized intermediates of six PCET steps of PC_6-Fe_4.

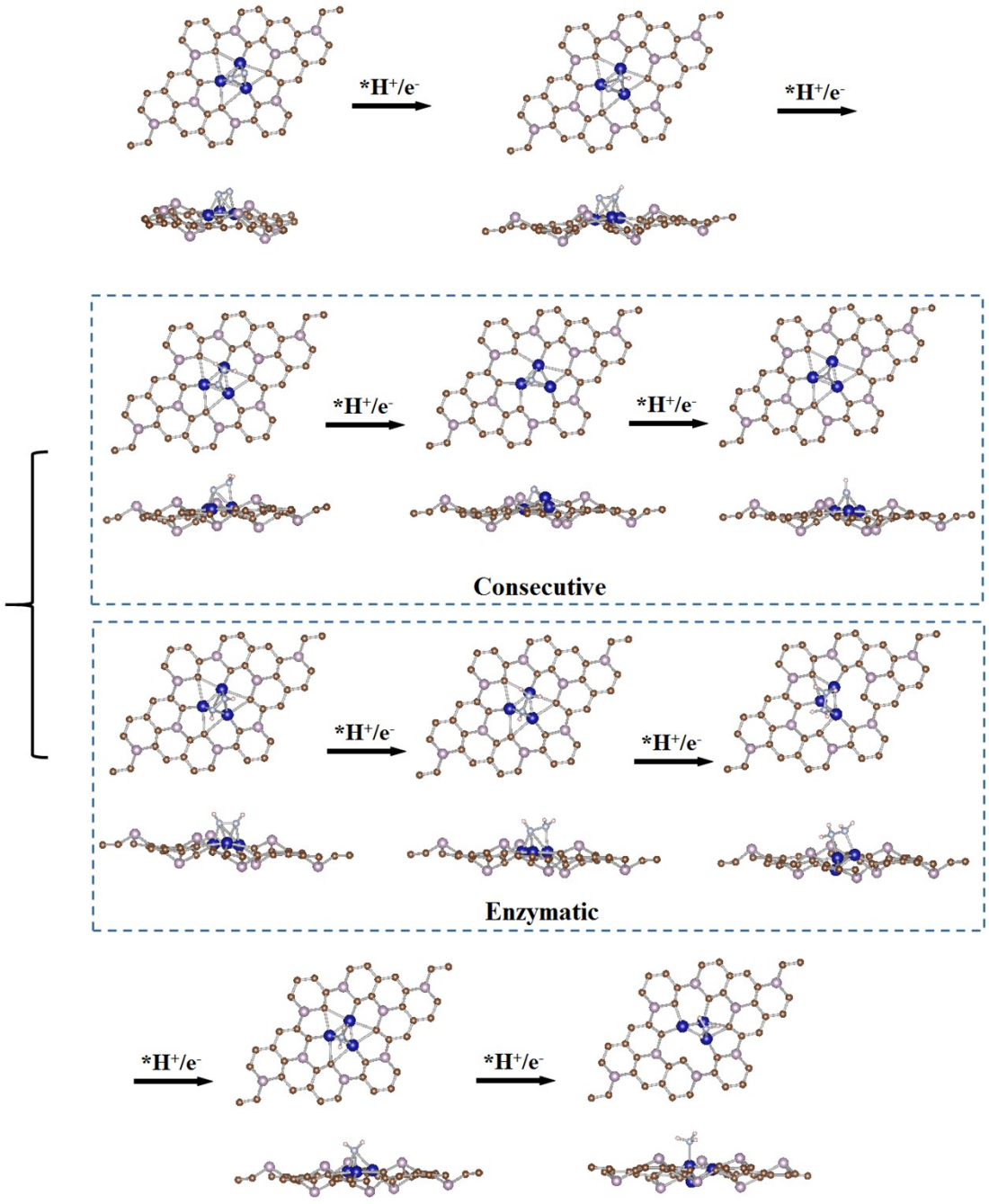

Fig. S5 The optimized intermediates of six PCET steps of PC_6-Cr_3.