Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

CO_2 Electroreduction Performance of Single Transition Metal Atom Supported on Porphyrin-Like Graphene: A Computational Study

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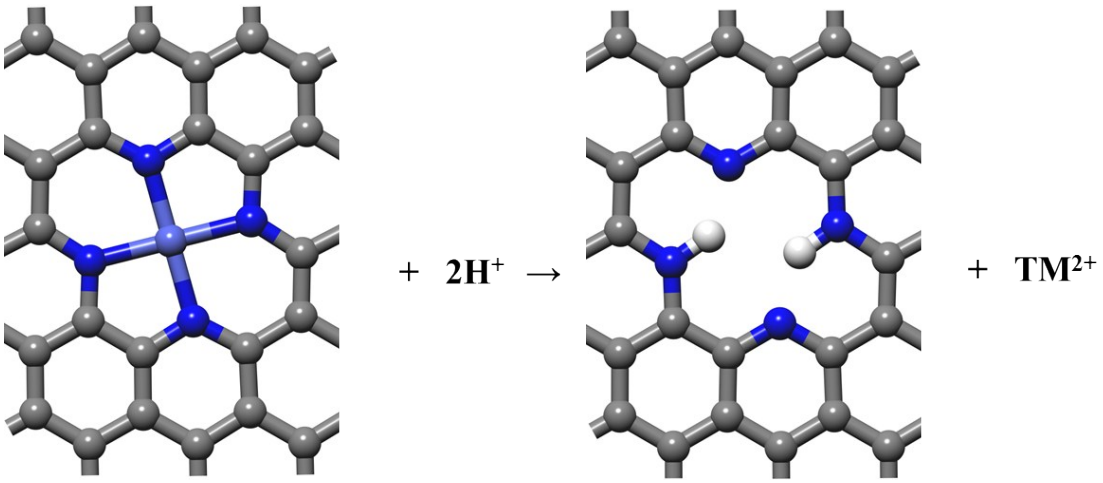
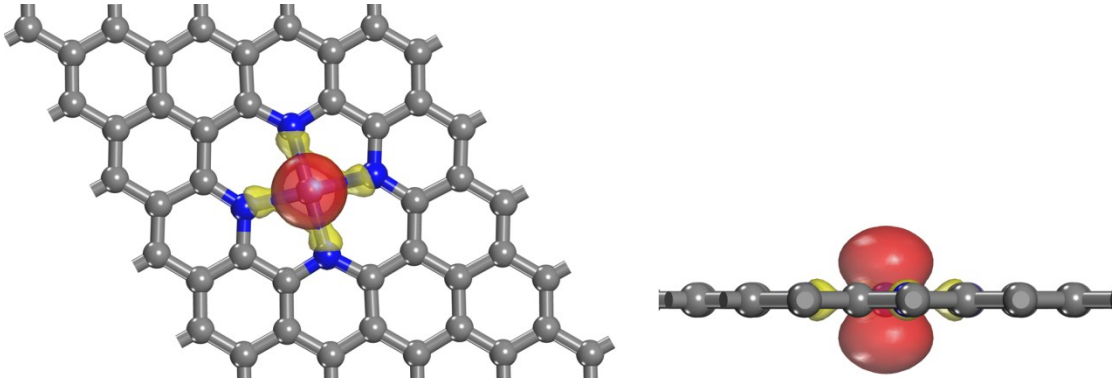


Fig. S1: Schematic diagrams of TM/H substitution reaction for single TM atom supported by porphyrin-like graphene.



(a) (b)

Fig. S2. The isosurface of spin-resolved density pictures of CoN_4-embedded graphene: (a) top and (b) side views. The isovalue is set to be 0.01 $eÅ^{-2}$.

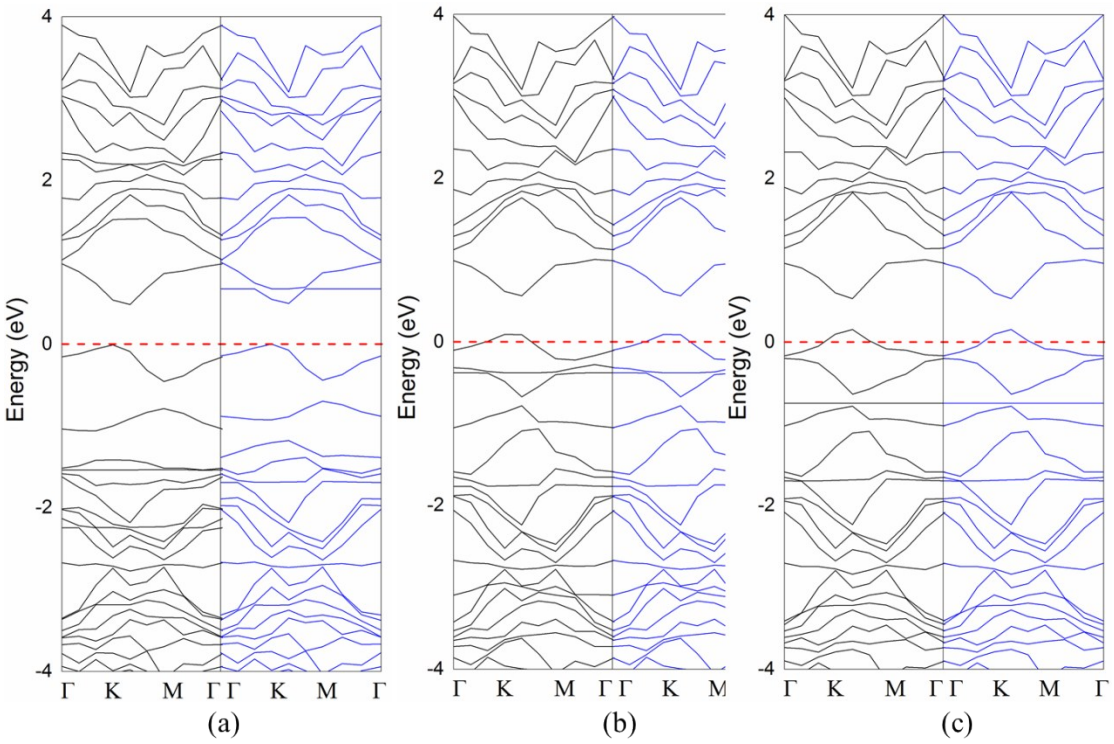
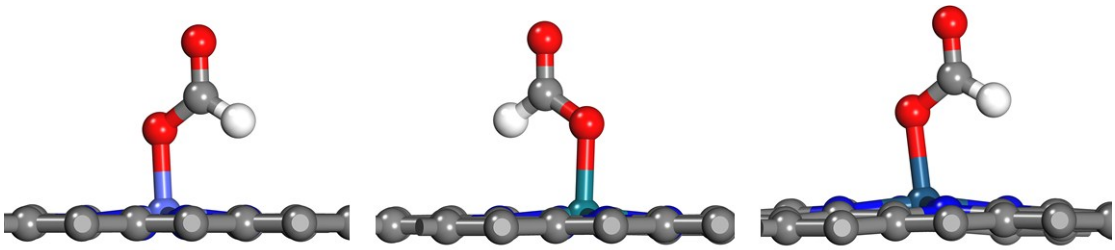


Fig. S3: The computed band structures of (a) CoN_4, (b) RhN_4, and (c) IrN_4 embedded graphenes. The Fermi level was set to zero as denoted by red dotted lines.



(a) (b) (c)

Fig. S4. Optimized structures of OCHO species on (a) Co, (b) Rh, and (c) Ir atoms supported by porphyrin-like graphene.