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SUPPLEMENTARY MATERIAL TO

Enhancing hydrogen evolution reaction using transition metal atoms on 6,6,12-graphyne: A DFT study

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Table S1. Detailed parameters for the optimized TM@GY structures. d_{TM-C} is the distance between the TM atom and its nearest acetylenic C atoms. Q refers to charges transferred from TM atoms to the substrate obtained by Hirshfeld charge analysis.

TM@GY	d_{TM-C} (Å)	Q (e)
Fe@GY	1.99	0.24
Co@GY	1.94	0.04
Ni@GY	1.95	0.03
Cu@GY	2.04	0.38

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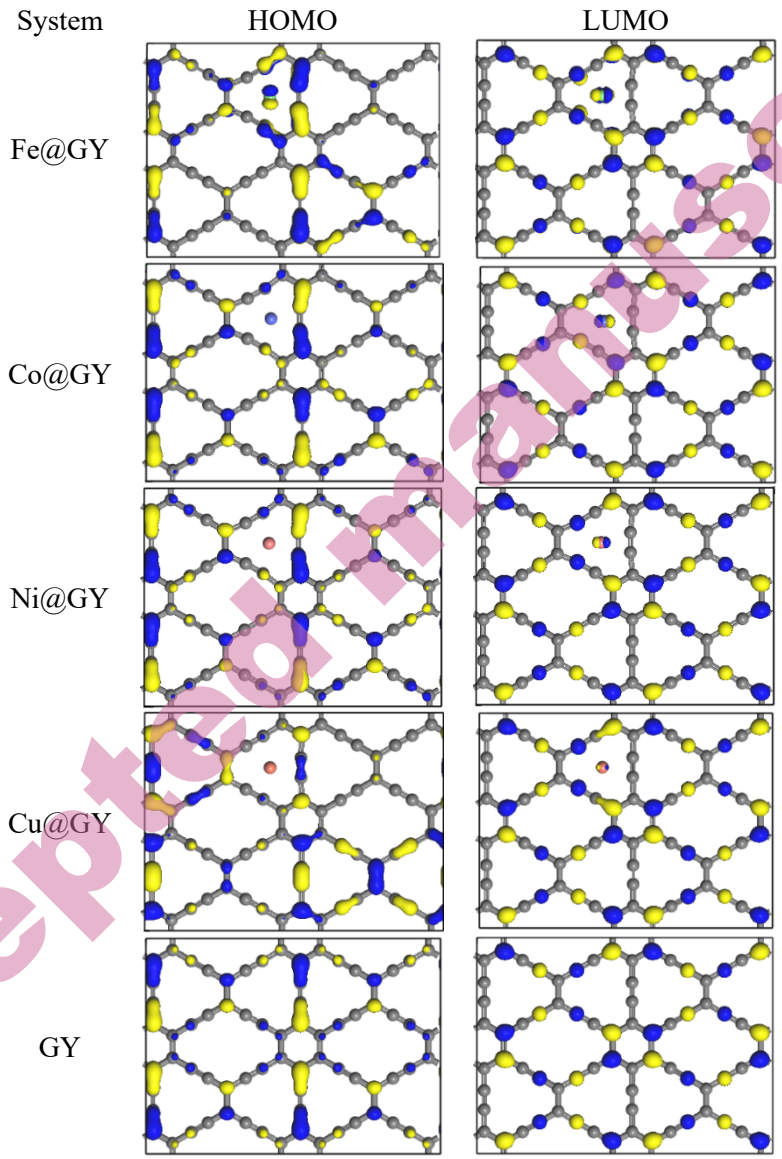

Fig. S1. Graphical representation of HOMOs and LUMOs of pristine and TM-decorated 6,6,12-graphyne nanosheets

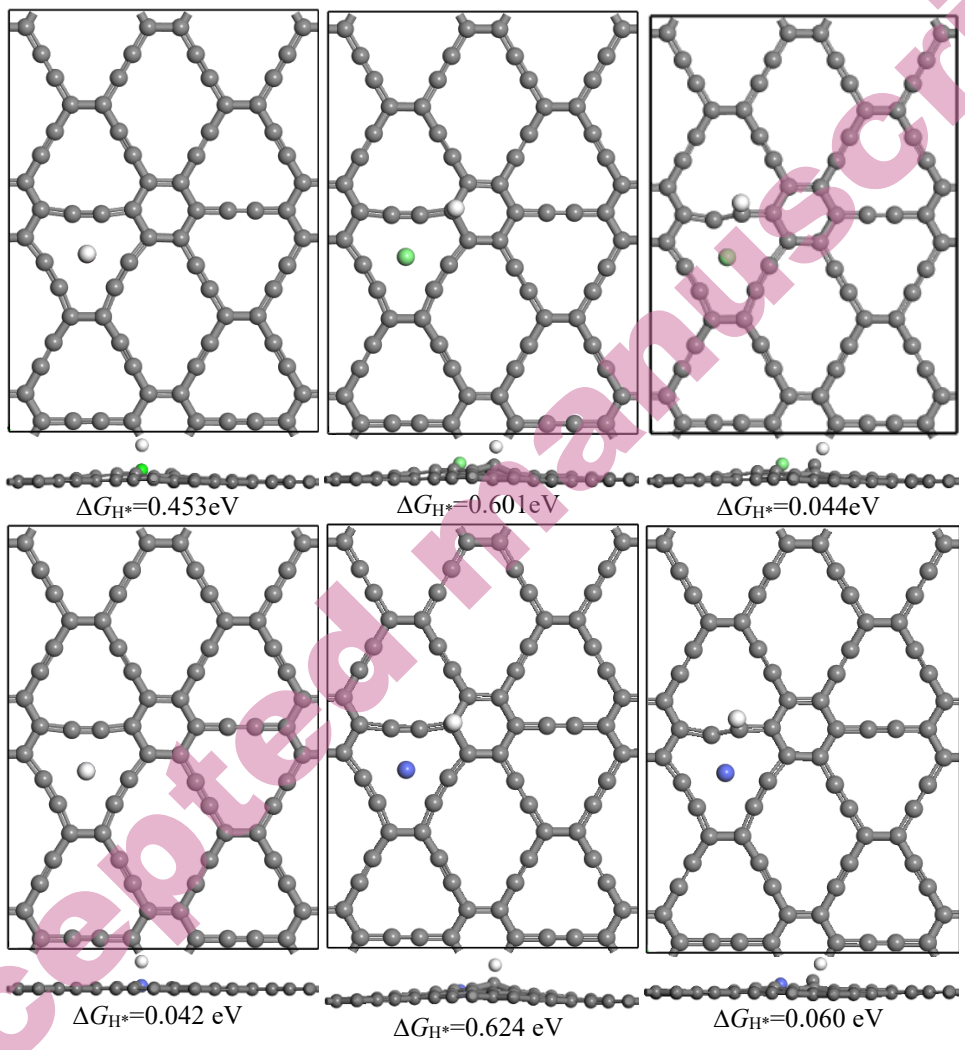

Fig. S2. Most stable adsorption configurations and corresponding adsorption free energies of *H on different sites of Fe@GY, Co@GY, Ni@GY, and Cu@GY. Grey, blue, green, yellow, orange, and white balls represent C, Co, Fe, Ni, Cu, and H, respectively

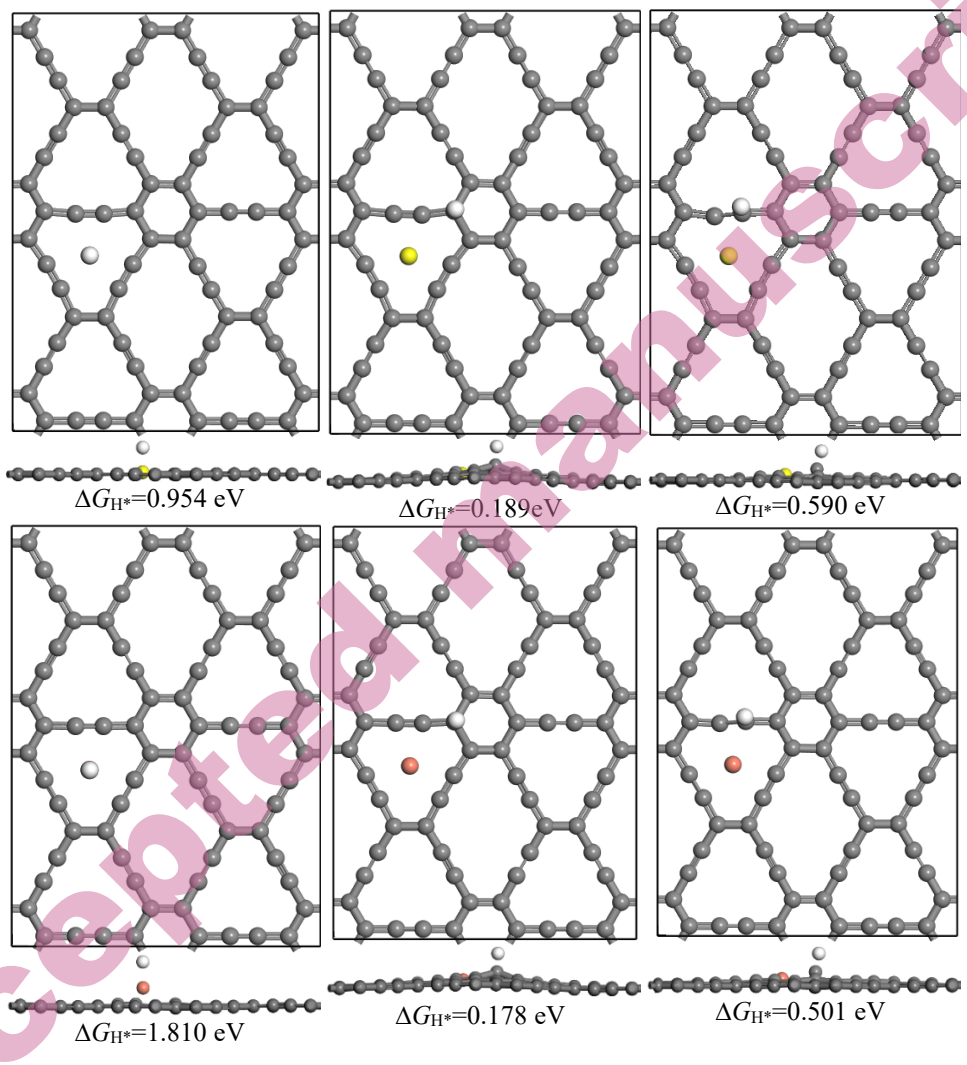

Fig. S2. Cont. Most stable adsorption configurations and corresponding adsorption free energies of *H on different sites of Fe@GY, Co@GY, Ni@GY, and Cu@GY. Grey, blue, green, yellow, orange, and white balls represent C, Co, Fe, Ni, Cu, and H, respectively

Table S2. Zero-point energy (ZPE) and entropic corrections (TS) in determining the free energy of reactants, intermediates, and products adsorbed on catalysts at 298 K. For the adsorbate, the ZPE value is not sensitive to the metal and coordination since they have close values.

Species	ZPE(eV)	TS(eV)
H_2	0.27	0.41
H*	0.16	0