Electronic Supplementary Material (ESI) for RSC Advances.

Density functional study on 3d metal/graphene for removing CO from H_2 feed gas in hydrogen fuel cells

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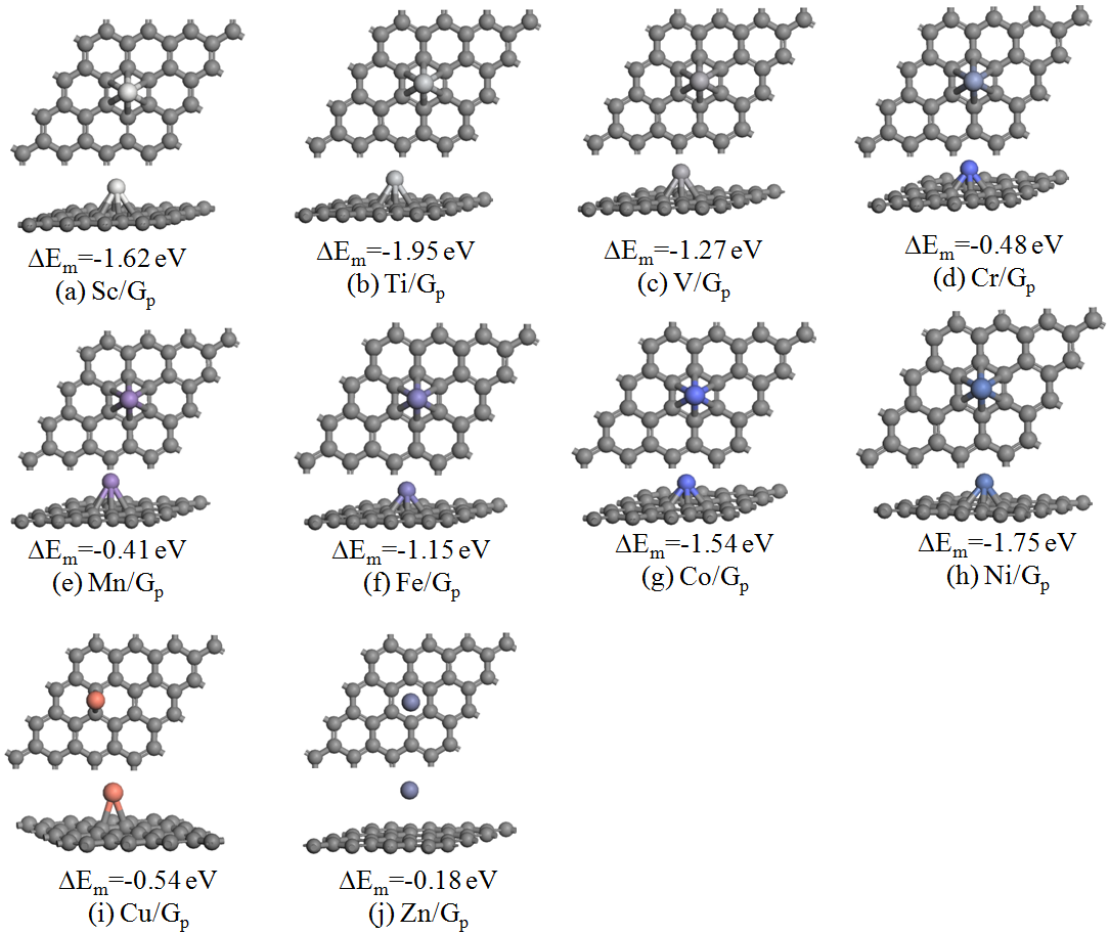

Fig. S1 The structures of metal atom (Sc - Zn) adsorption on perfect graphene G_p. ΔE_m denotes the adsorption energy of metal atom on graphene.

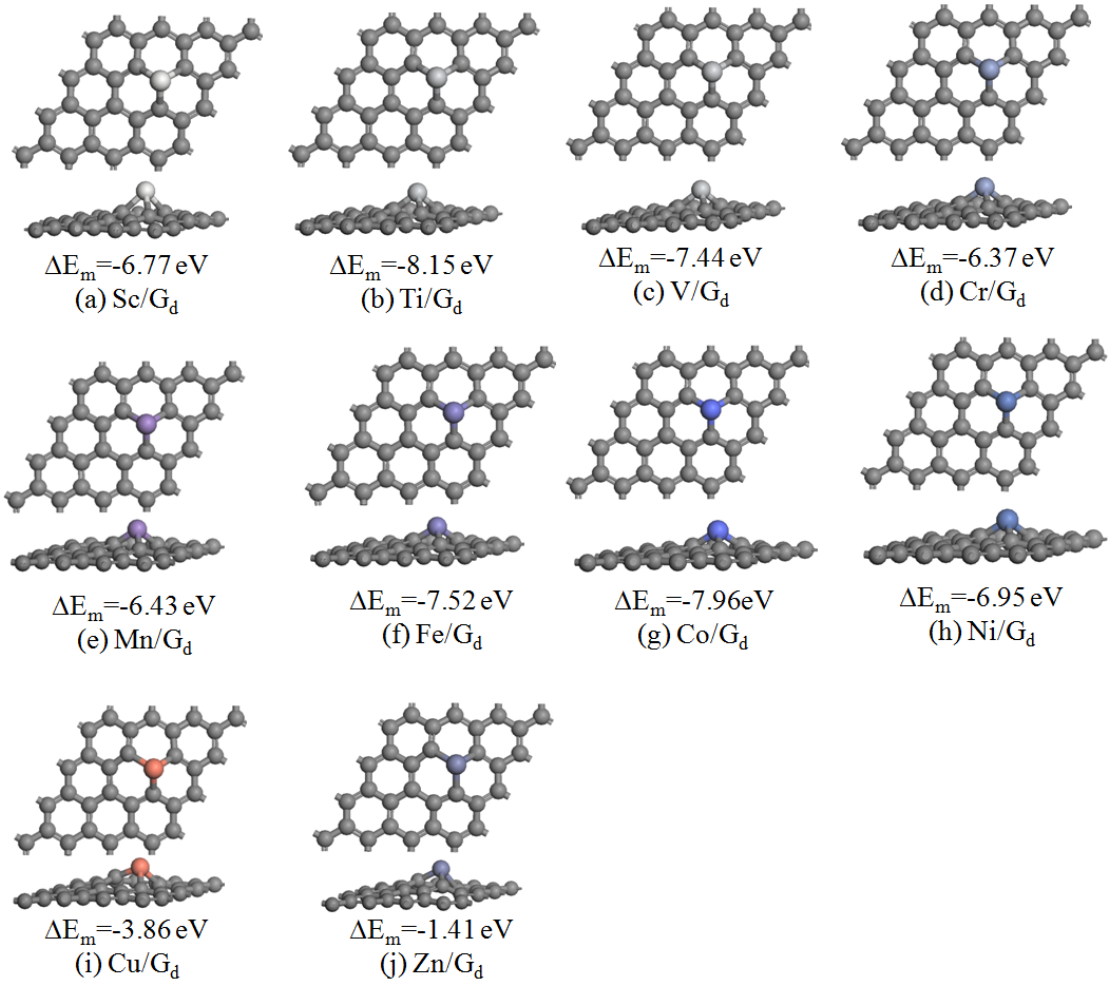

Fig. S2 The structures of metal atom (Sc - Zn) adsorption on defect graphene G_d.

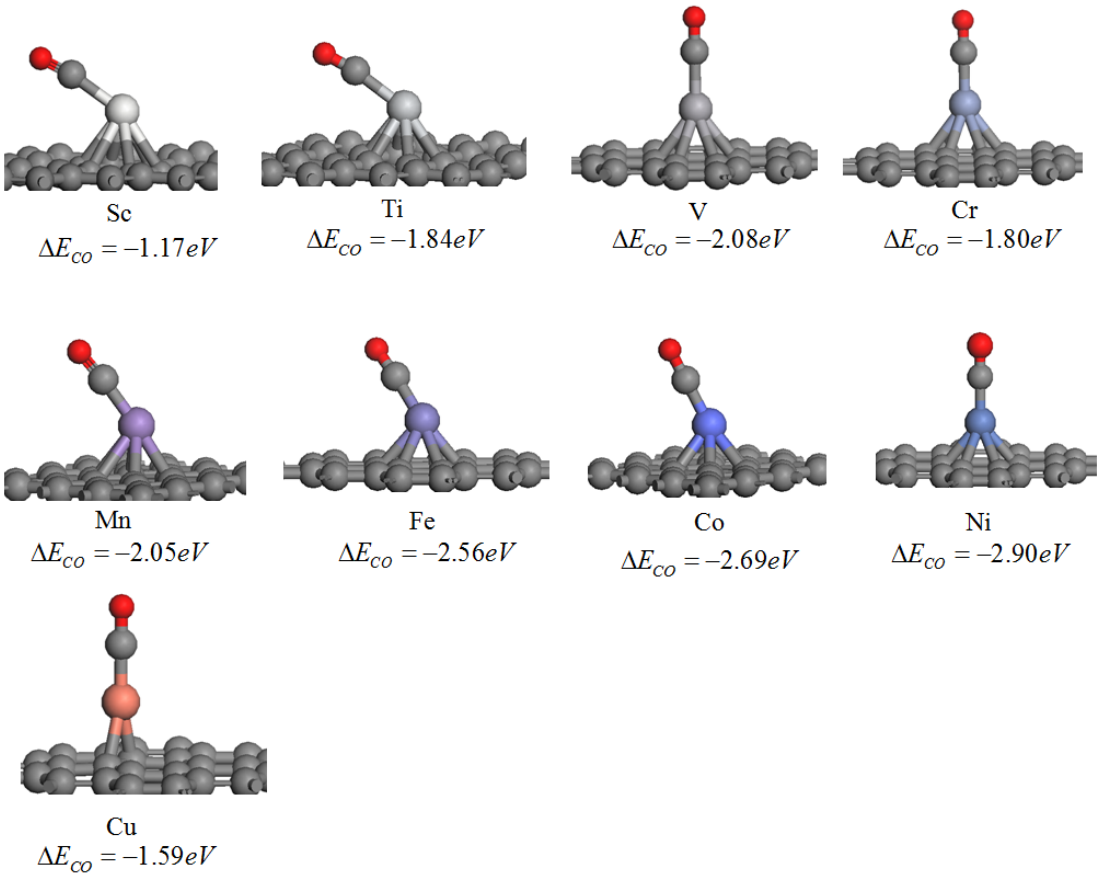

Fig. S3 The structures of CO adsorption on M/G_p. The gray and red balls denote the carbon and O atom, respectively. ΔE_{CO} denotes the adsorption energy of CO.

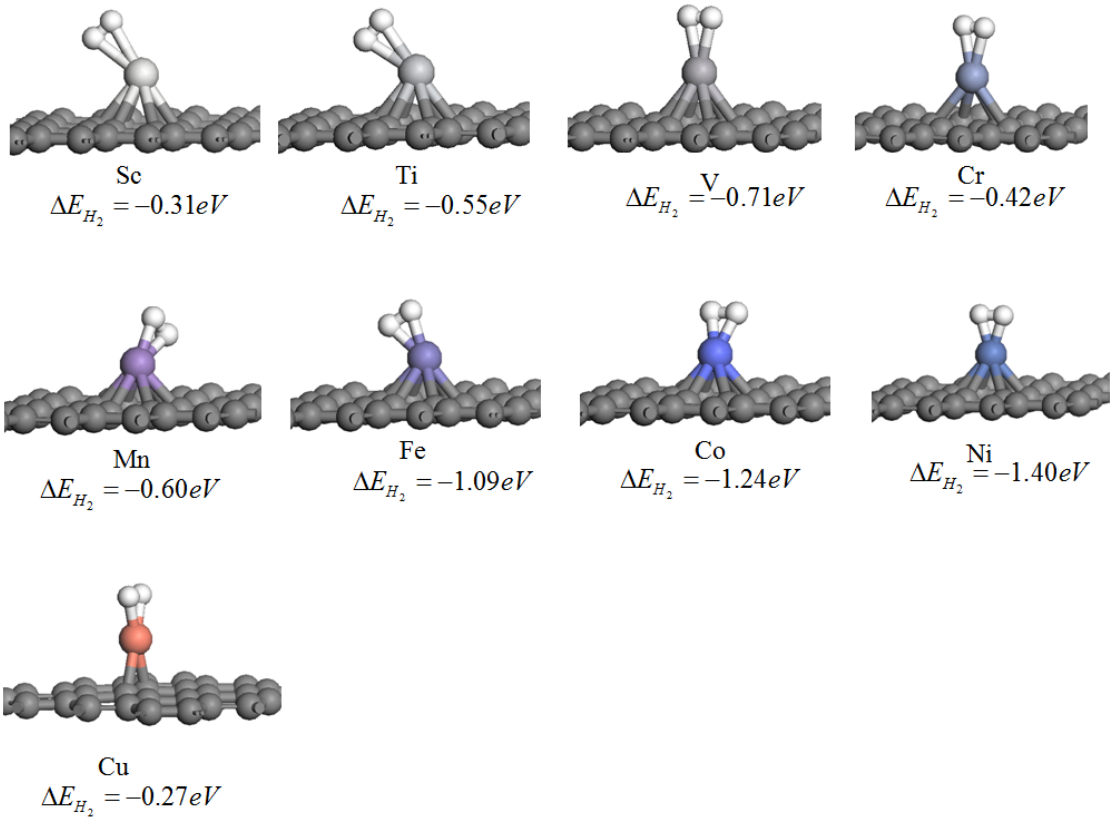

Fig. S4 The structures of H_2 adsorption on M/G_p. The gray and red balls denote the carbon and O atom, respectively. ΔE_{H_2} denotes the adsorption energy of H_2.

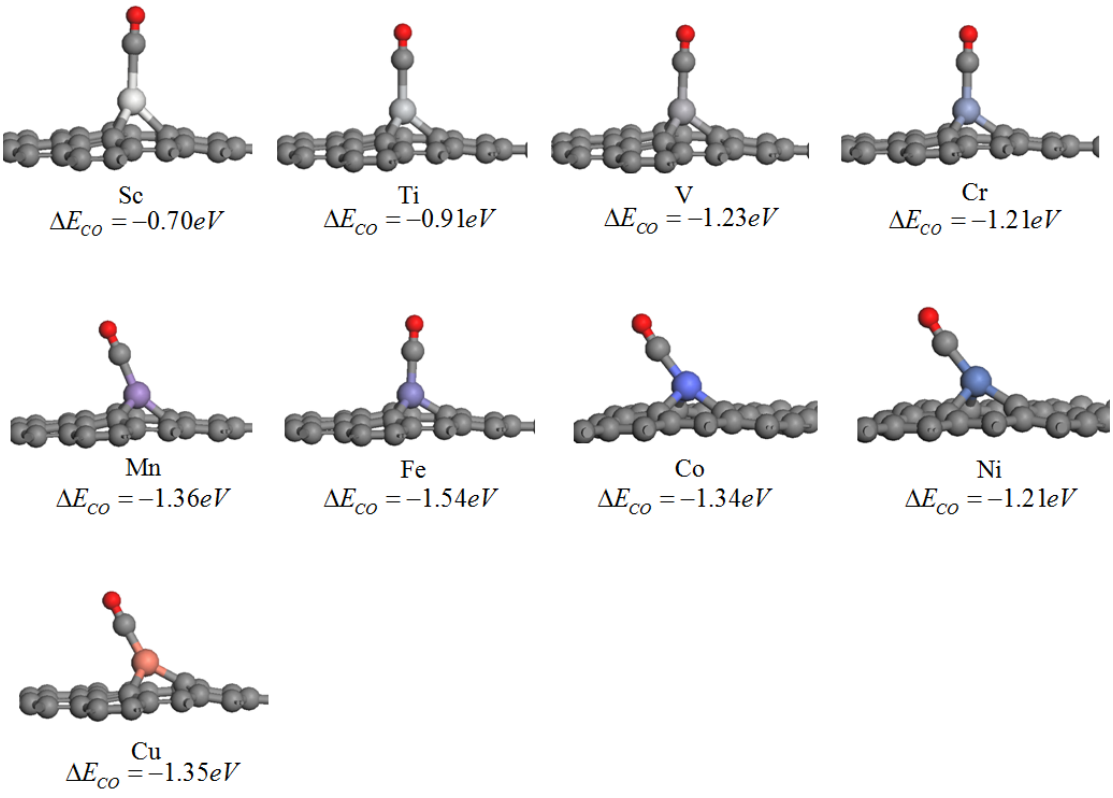

Fig. S5 The structures of CO adsorption on M/G_d. The gray and red balls denote the

carbon and O atom, respectively.

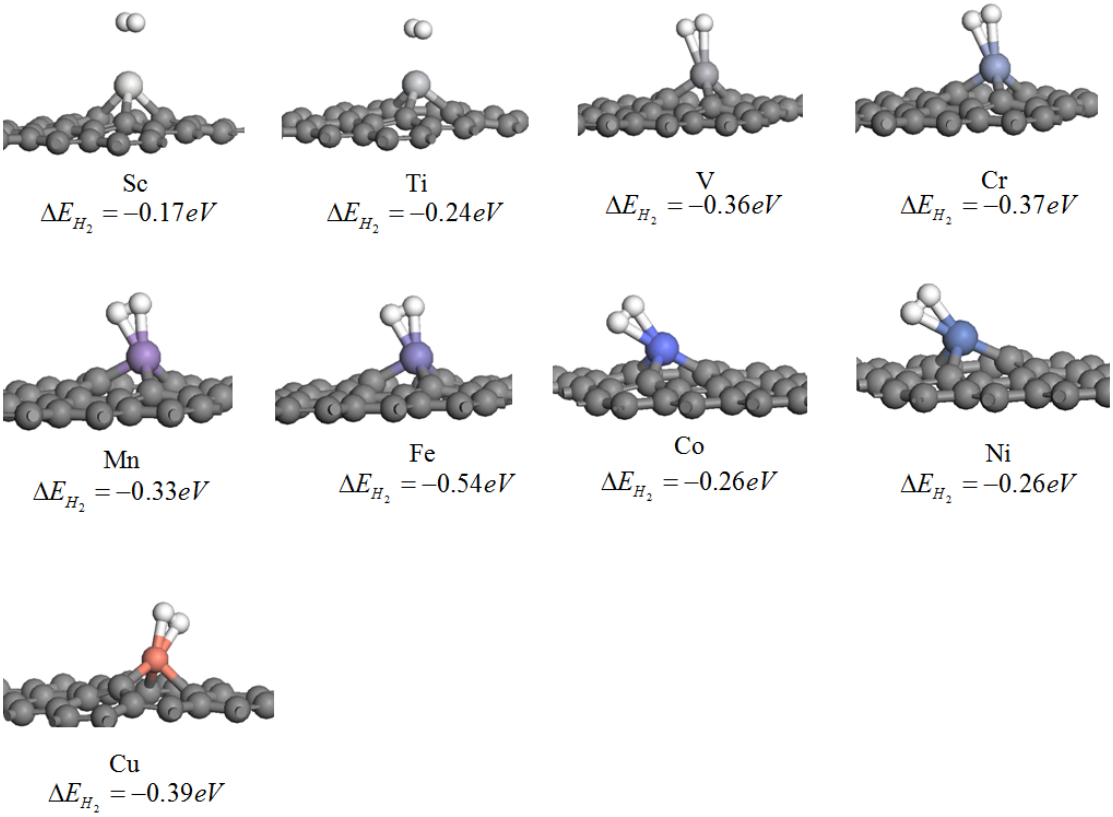

Fig. S6 The structures of H_2 adsorption on M/G_d. The gray and red balls denote the carbon and O atom, respectively.