

Electronic Supplementary Information

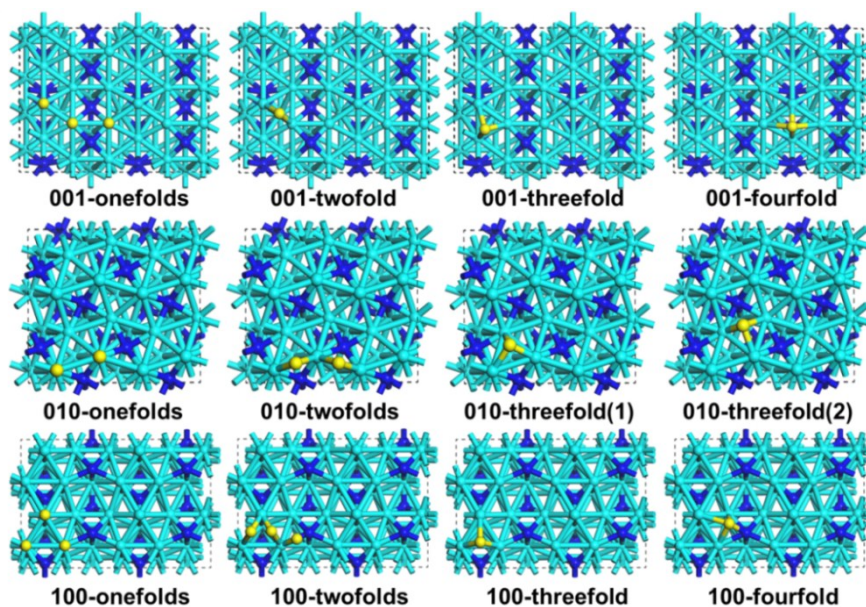


Figure S1- Adsorption structures of carbon on Fe_3C : Fe and C and adsorbed C atoms are in green, blue, and yellow, respectively ^[16]

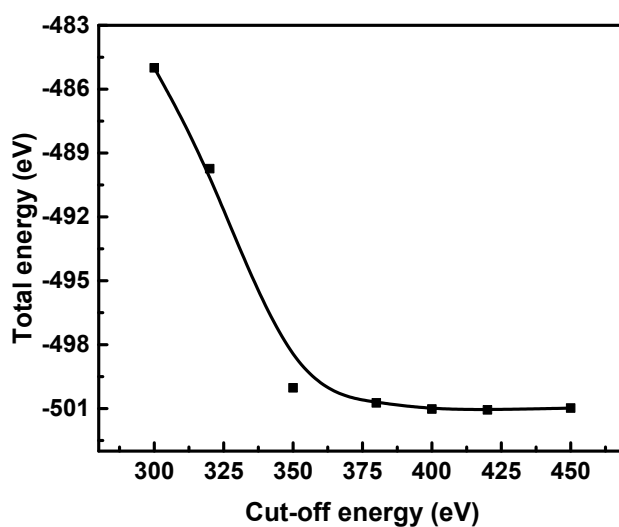


Figure S2 - convergence tests for cut-off energy (Fe_3C slab system)

Table S1- convergence tests for k-points sampling

Cut-off energy	k-points	Total energy (eV)
400 eV	8×6×9	-135.3382
	9×6×10	-135.3401
	9×7×11	-135.3404
	10×7×11	-135.3404
	10×8×12	-135.3405
	11×8×12	-135.3407
	12×9×13	-135.3407
	12×9×14	-135.3403

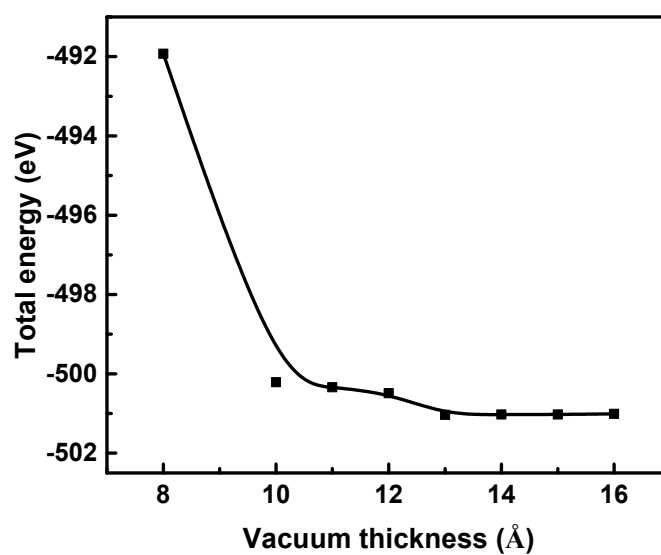


Figure S3- convergence tests for vacuum thickness