Supplementary Information

Enhancing lithium storage performance with silicon-based anodes: a theoretical study on transition metal-integrated SiO_x/M@C (M = Fe, Co, Ni) heterostructures

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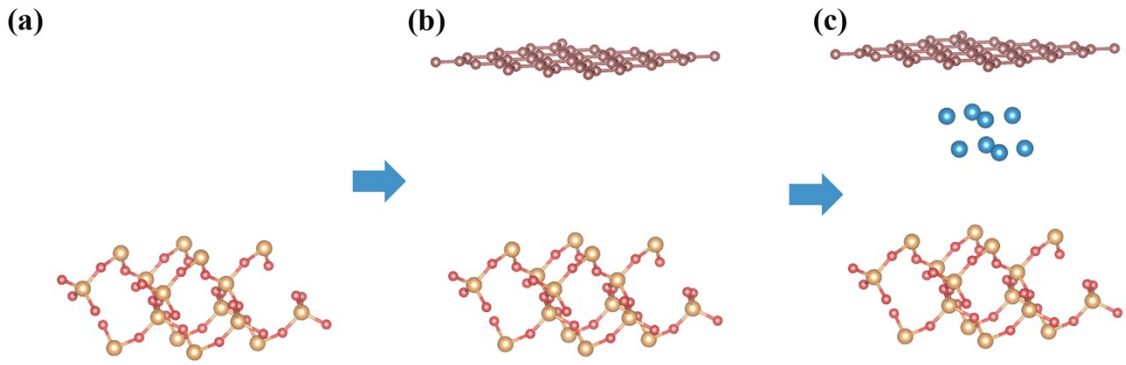

Fig. S1 Geometrically optimized structures of (a) SiO_2; (b) SiO_2@C; (c) SiO_2/M@C.

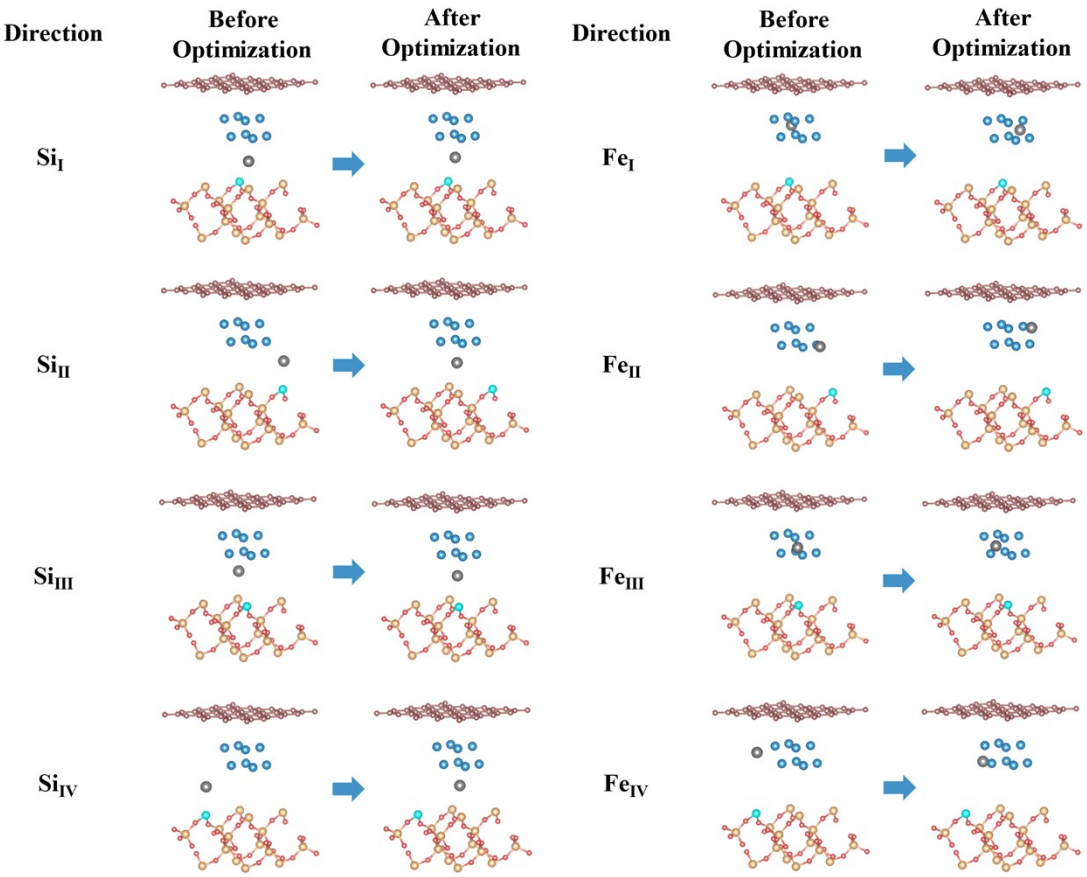

Fig. S2 Configurations before and after optimization of all directions for SiO_x/Fe@C.

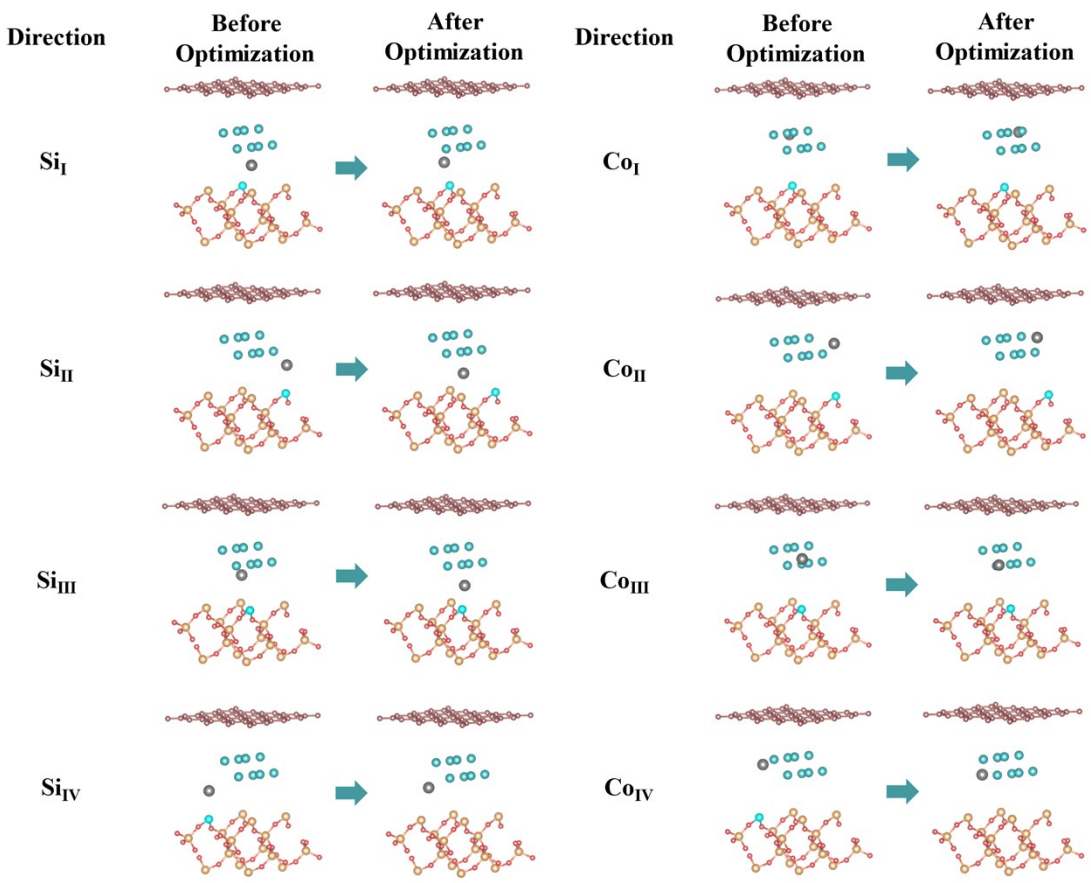

Fig. S3 Configurations before and after optimization of all directions for SiO_x/Co@C.

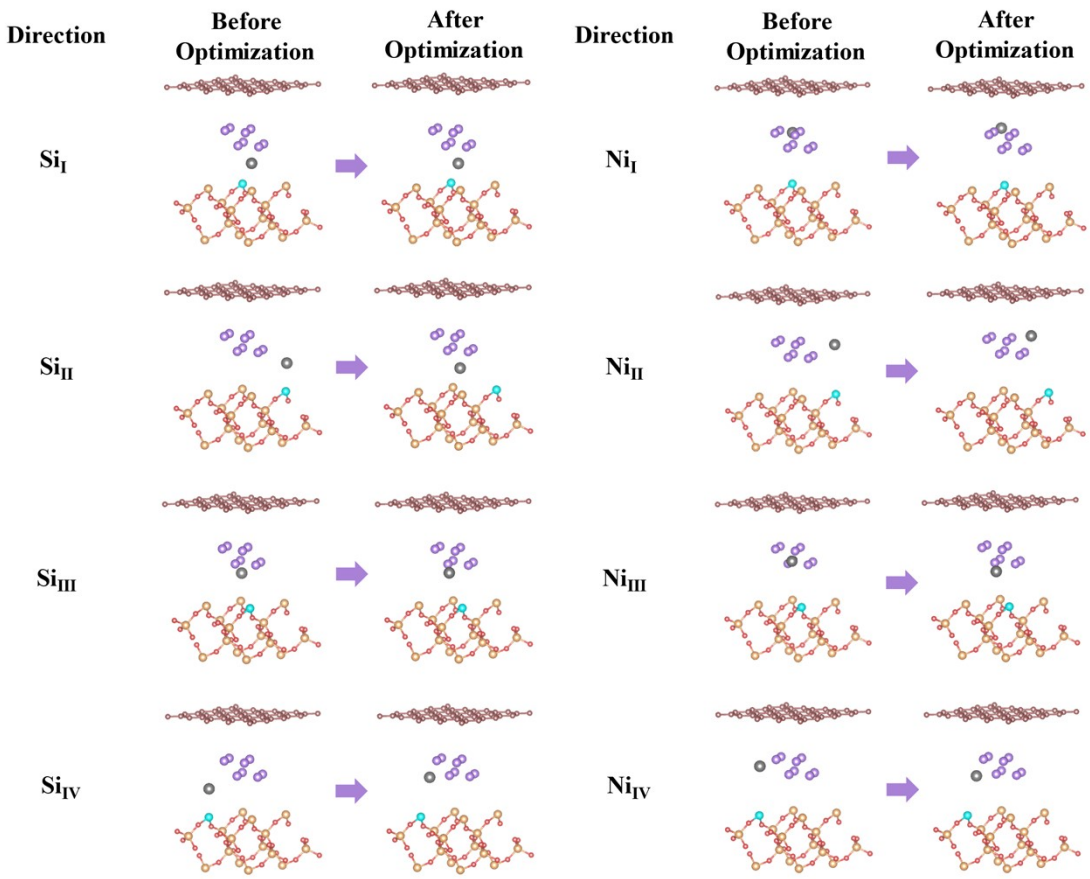

Fig. S4 Configurations before and after optimization of all directions for SiO_x/Ni@C.

Table S1 The energies of $E(SiOx/M@C), E(SiOx@C), and\ E(M)$.

Compound	Energy/eV
SiO_x/Fe@C	-24099.0845
SiO_x/Co@C	-25524.3973
SiO_x/Ni@C	-28019.2597
SiO_x@C	-17200.865
Fe	-6913.93799
Co	-8327.92068
Ni	-6901.50753
Li	-188.143764

Table S2 The energies of $E(Li + SiOx/M@C)$.

Material	Direction	ΔEa/eV	Direction	ΔEa/eV
Li+SiO_x/Fe@C	Si_I	-24289.6282	Fe_I	-24289.5908
	Si_{II}	-24289.6282	Fe_{II}	-24289.3222
	Si_{III}	-24289.6281	Fe_{III}	-24289.6031
	Si_{IV}	-24289.6288	Fe_{IV}	-24289.6031
Li+SiO_x/Co@C	Si_I	-25714.9522	Co_I	-25714.9236
	Si_{II}	-25715.0467	Co_{II}	-25714.9237
	Si_{III}	-25715.0462	Co_{III}	-25714.9239
	Si_{IV}	-25714.6591	Co_{IV}	-25714.9218
Li+SiO_x/Ni@C	Si_I	-28210.2236	Ni_I	-28209.6864
	Si_{II}	-28210.1111	Ni_{II}	-28209.9026
	Si_{III}	-28209.8913	Ni_{III}	-28209.8906
	Si_{IV}	-28209.9019	Ni_{IV}	-28209.9022