Can NOx reduction by CO react over carbon-based single-atom catalysts at low temperatures? A theoretical study

Jie Shi[1], Wei Zhang[1], Yuan Pu[1], Hui Li[1], Dan Wang[1], and Jianfeng Chen[1]

[1]Beijing University of Chemical Technology

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Abstract

First principles studies combined with the microkinetic analysis were performed to study the reliability and reaction mechanisms of single-atom doped graphene (SADGr) materials in catalyzing NOx reduction with CO. By screening the 3d transition metals (Sc-Zn) and group-IV elements (Si and Ge), it was found that the Ti and Co doped graphene sheets (TiGr and CoGr) respectively own excellent catalytic activities in the NO/NO2-to-N2O and the N2O-to-N2 processes at low temperatures. Therefore, the TiGr/CoGr composite can be a promising catalyst in NOx reduction with CO. It was further revealed the combination of adsorption energy and electronegativity was a good descriptor to predict the activation energies. The obtained results can provide useful information for rational design of carbon-based single-atom catalysts for NOx reduction by CO at low temperatures.

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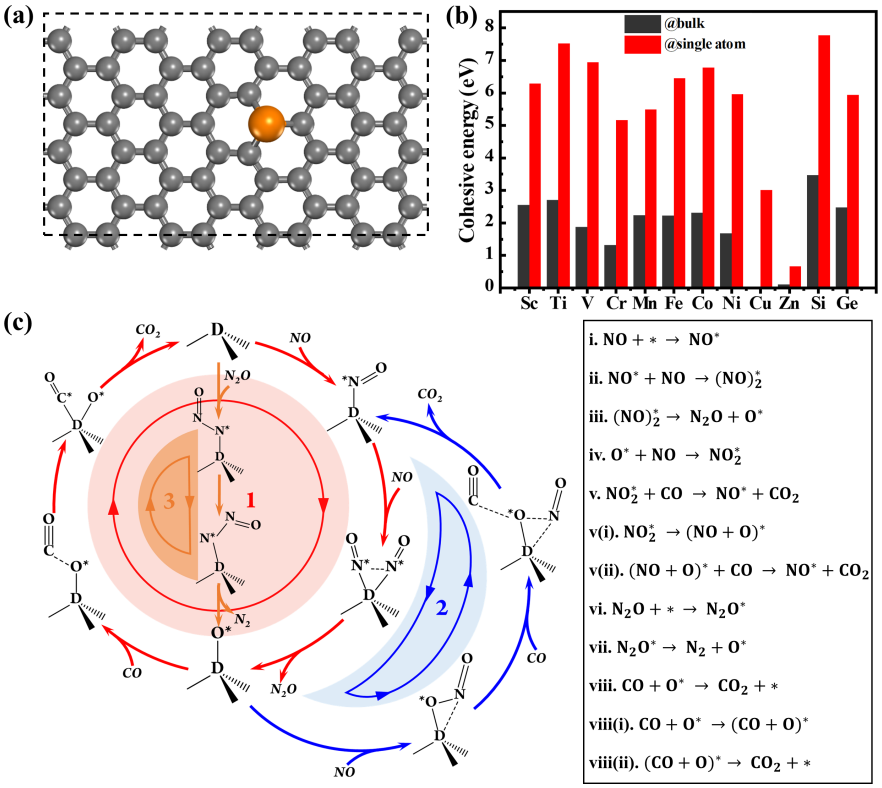

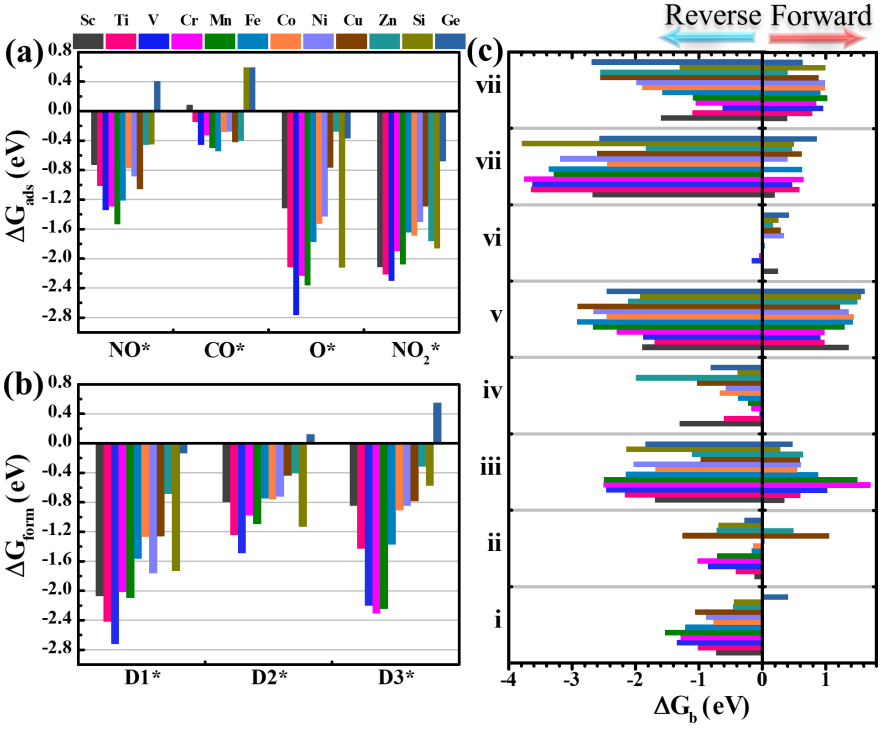

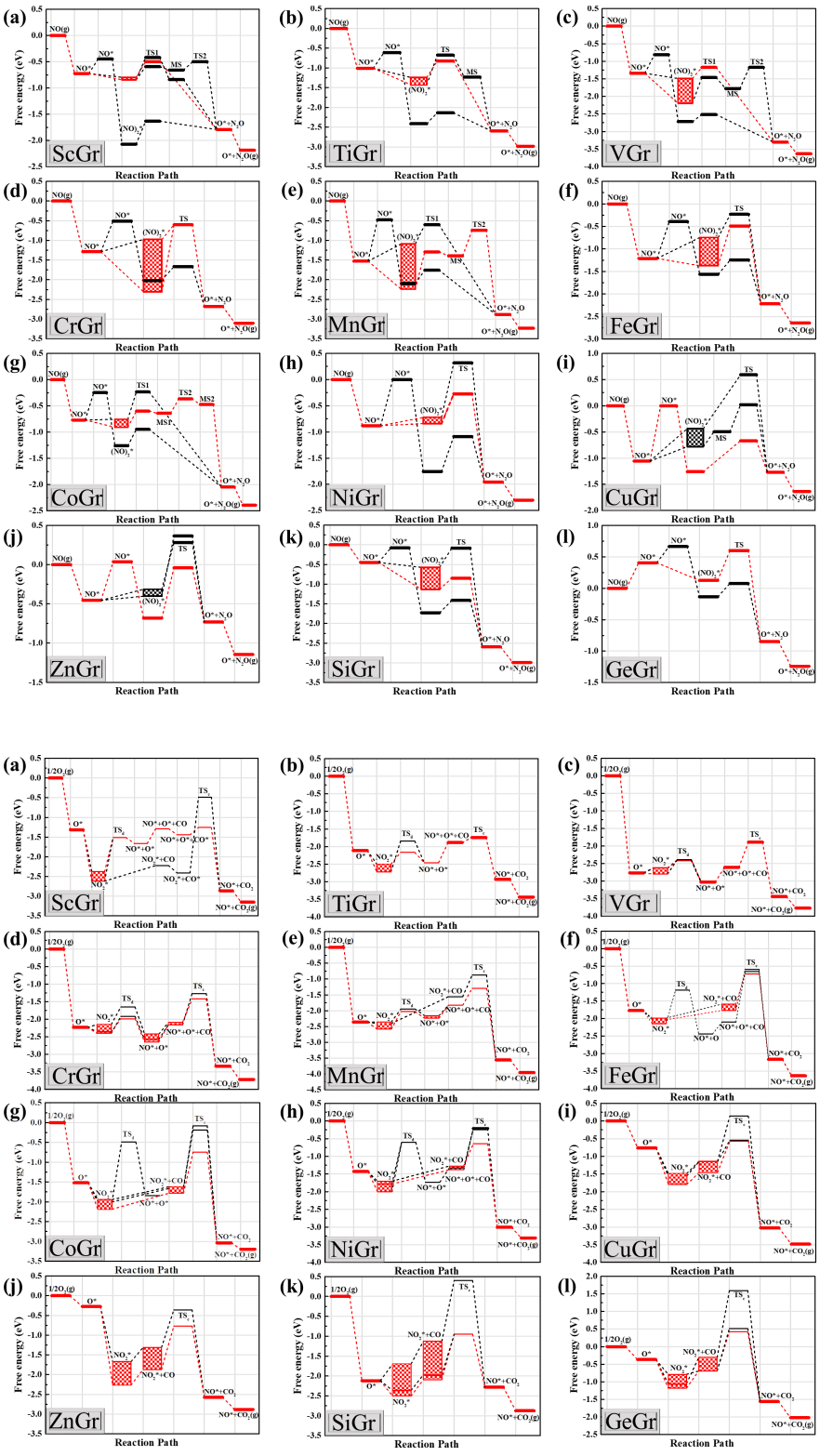

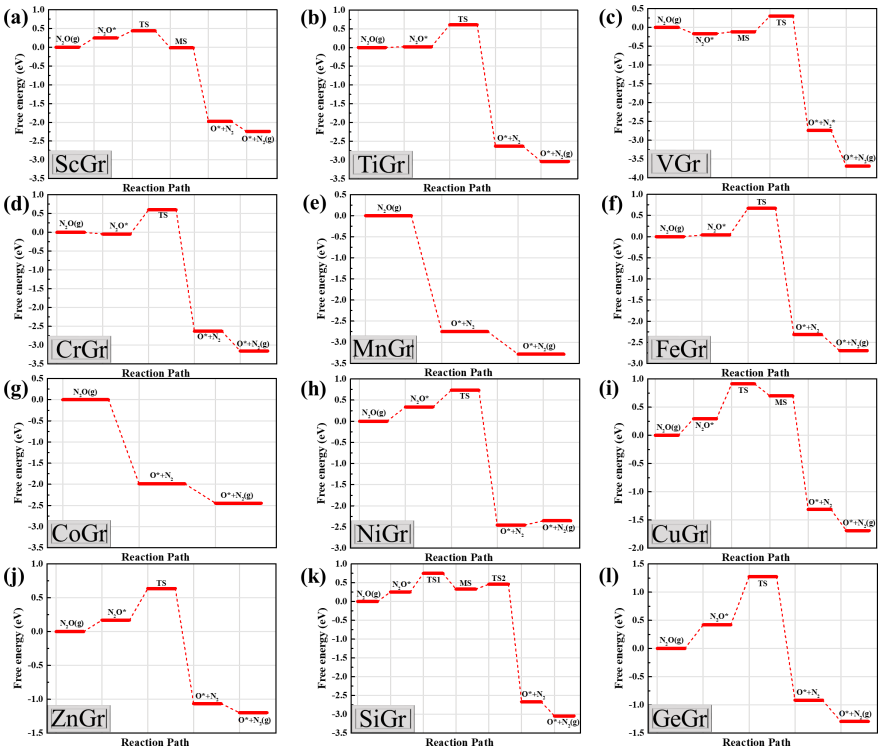

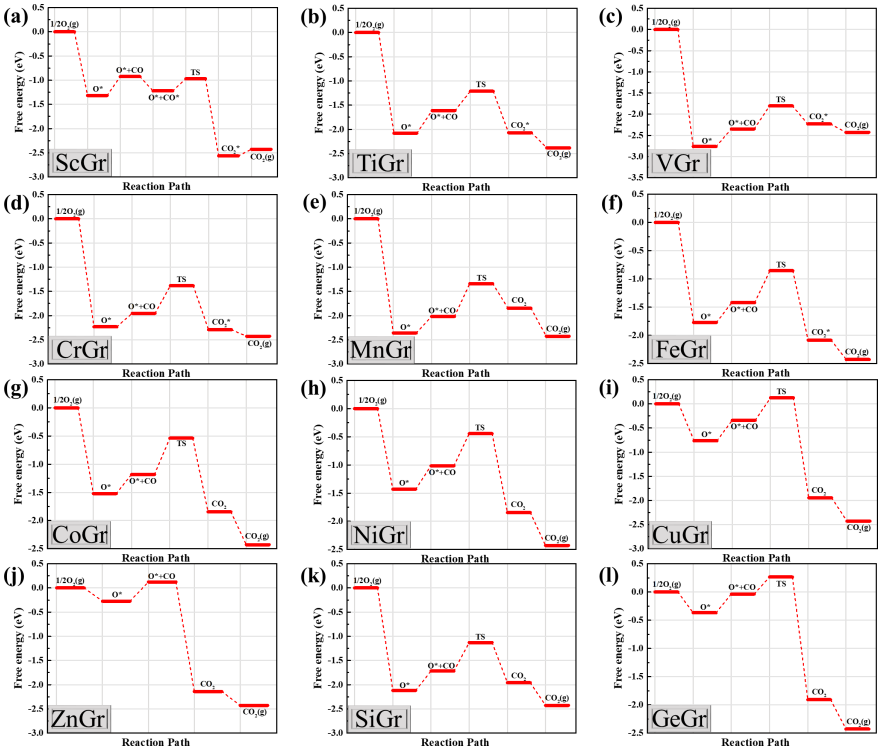

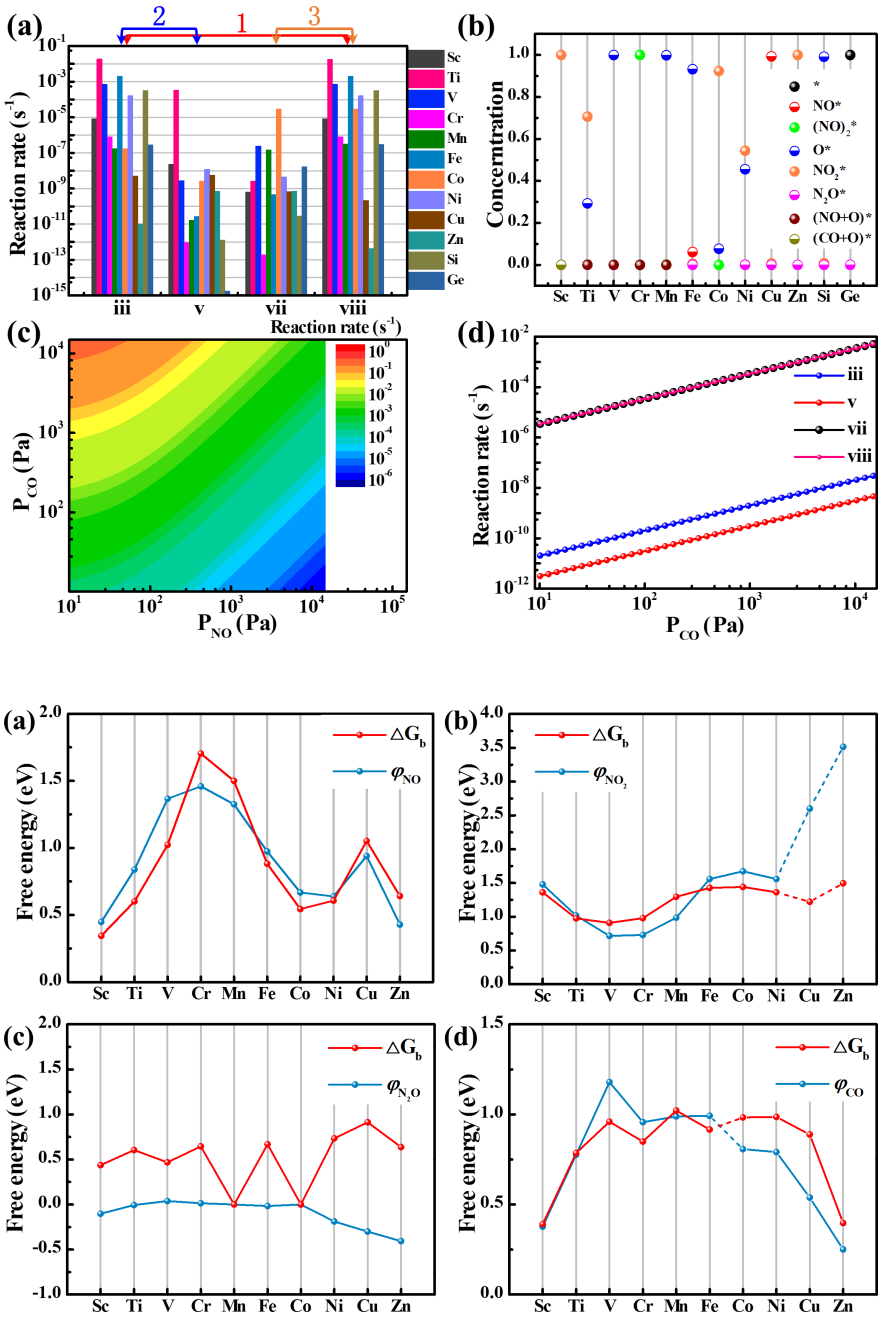

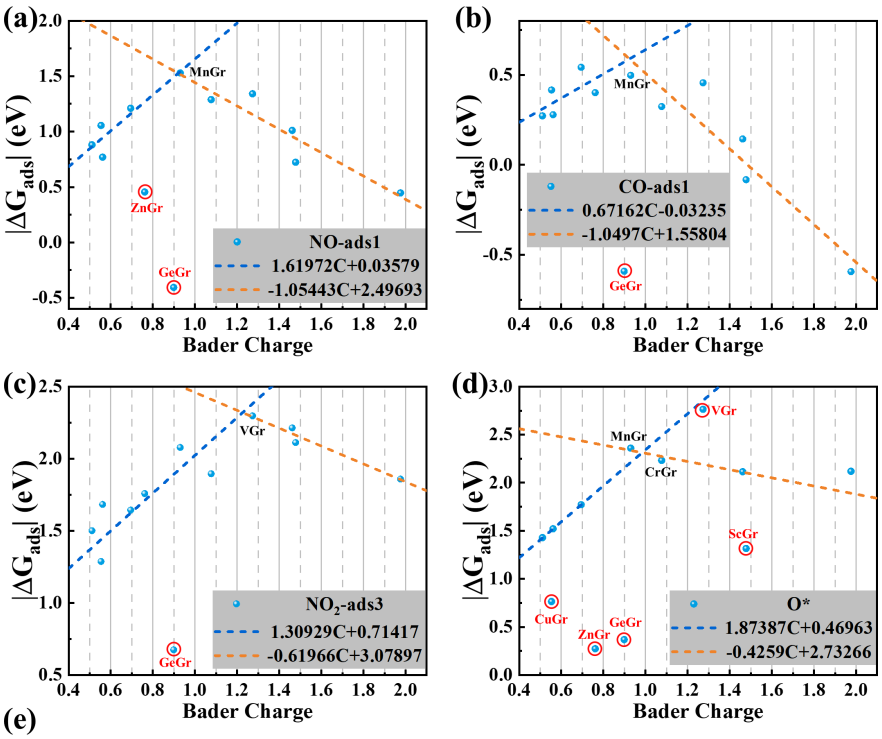

(e)

SADGr	NiGr	CuGr	CoGr	FeGr	ZnGr	GeGr	MnGr	CrGr	VGr	TiGr	ScGr	SiGr
Charge	0.511	0.554	0.561	0.695	0.761	0.899	0.93	1.077	1.273	1.462	1.478	1.976