Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Single silicon-doped CNT as a metal-free electrode for robust nitric oxide reduction utilizing a Lewis base site: An ingenious electronic "Reflux-Feedback" mechanism

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Figure S1. The transition state search of NORR on Si-CNT(10, 0).

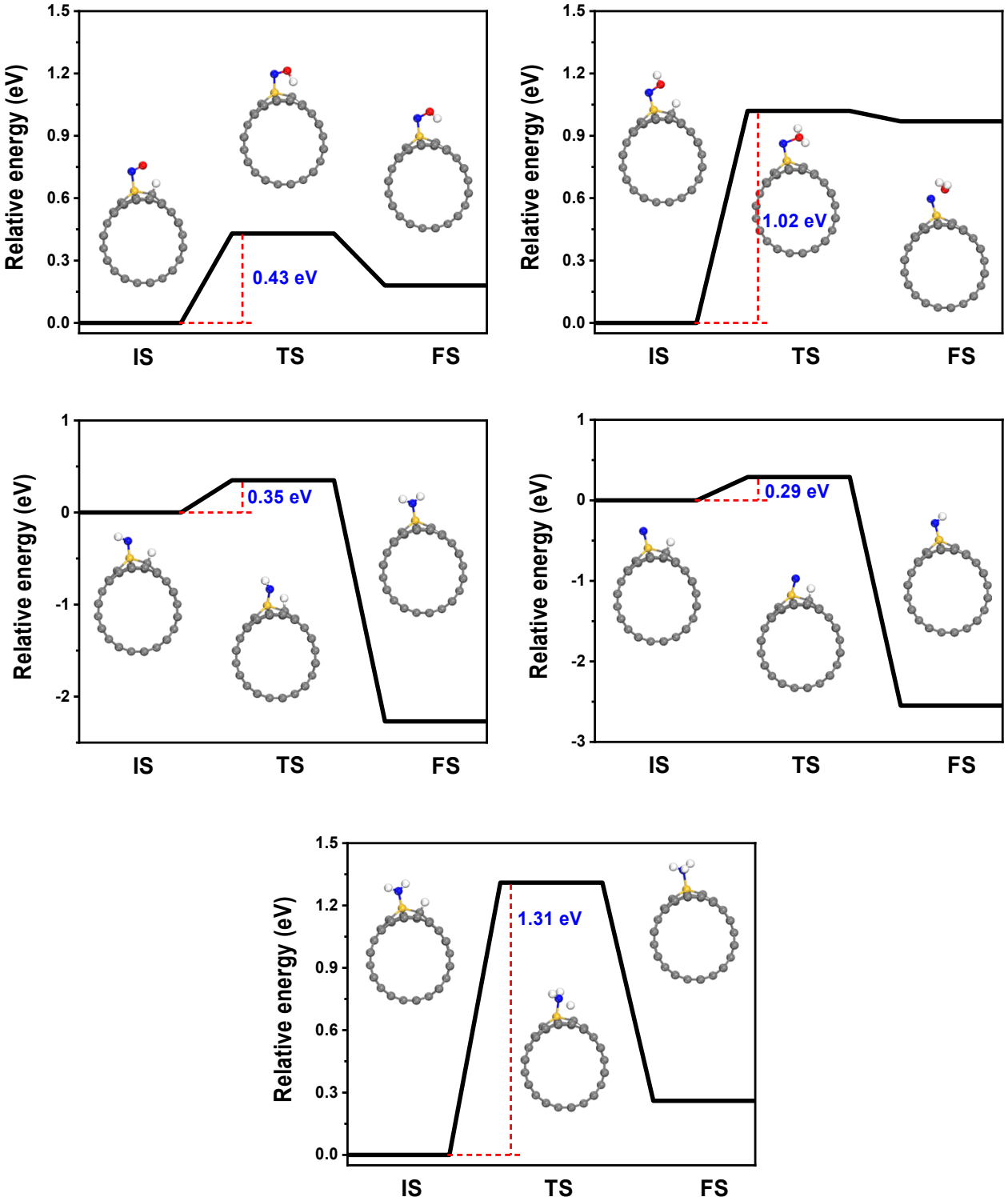

Table S1. The adsorption energy of NO with O-end, N-end and side on adsorption modes. (eV)

Systems	O-end	N-end	Side on
Si-G	-0.34	-0.80	
Si-CNT(6, 0)	-0.05	-0.96	
Si-CNT(7, 0)	-0.02	-0.90	
Si-CNT(8, 0)	0.00	-0.89	
Si-CNT(9, 0)	-0.05	-0.85	
Si-CNT(10, 0)	-0.08	-0.83	
Si-CNT(11, 0)	-0.08	-0.83	
Si-CNT(12, 0)	-0.07	-0.81	

Table S2. The adsorption free energy changes of NORR on Si-CNT(10, 0) with and without solvent effect. (eV)

	With solvent effect	Without solvent effect
*NO	-0.88	-0.85
*NOH	-0.82	-0.75
*N	-0.67	-0.57
*NH	-2.77	-2.60
$*NH_2$	-4.70	-4.90
$*NH_3$	-4.48	-4.64
U_L	-0.22	-0.25