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Single Tungsten Atom Supported on N-Doped γ-graphyne as a High-Performance Electrocatalyst for Nitrogen Fixation under Ambient Conditions

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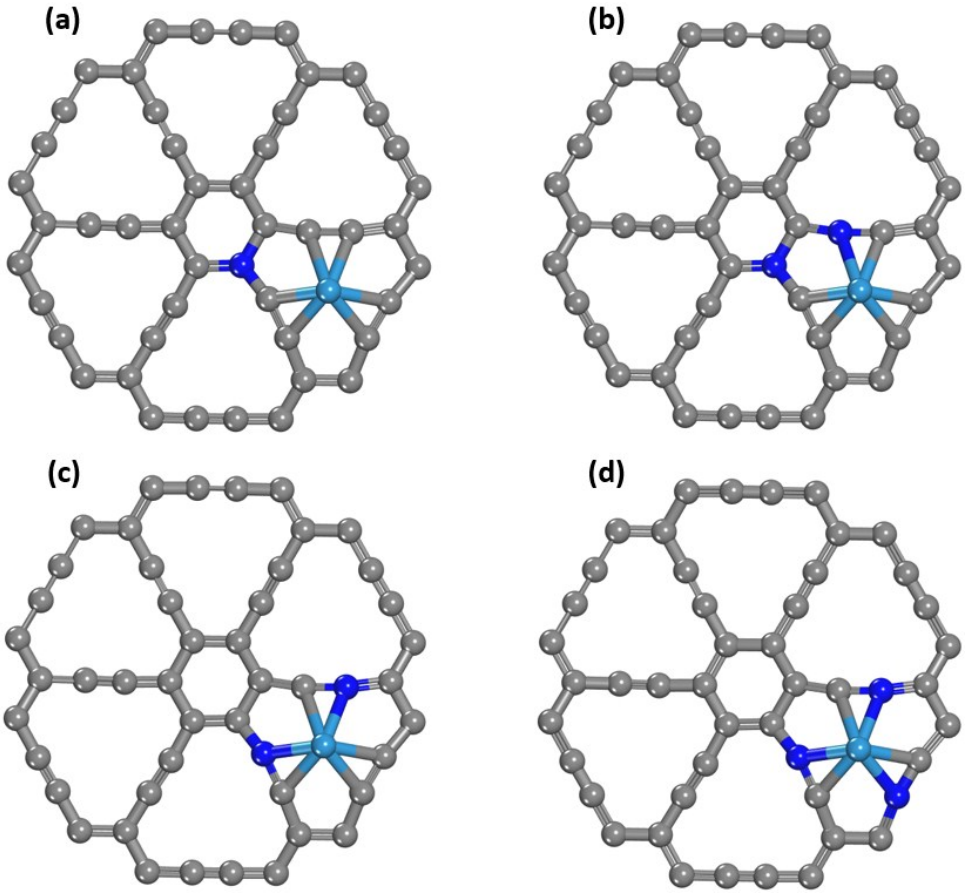

Figure S1. Structures of WN_x with (a) WN_1, (b) and (c) WN_2 and (d) WN_3 active centers. Gray, cyan and blue balls represent the C, W and N atoms, respectively.

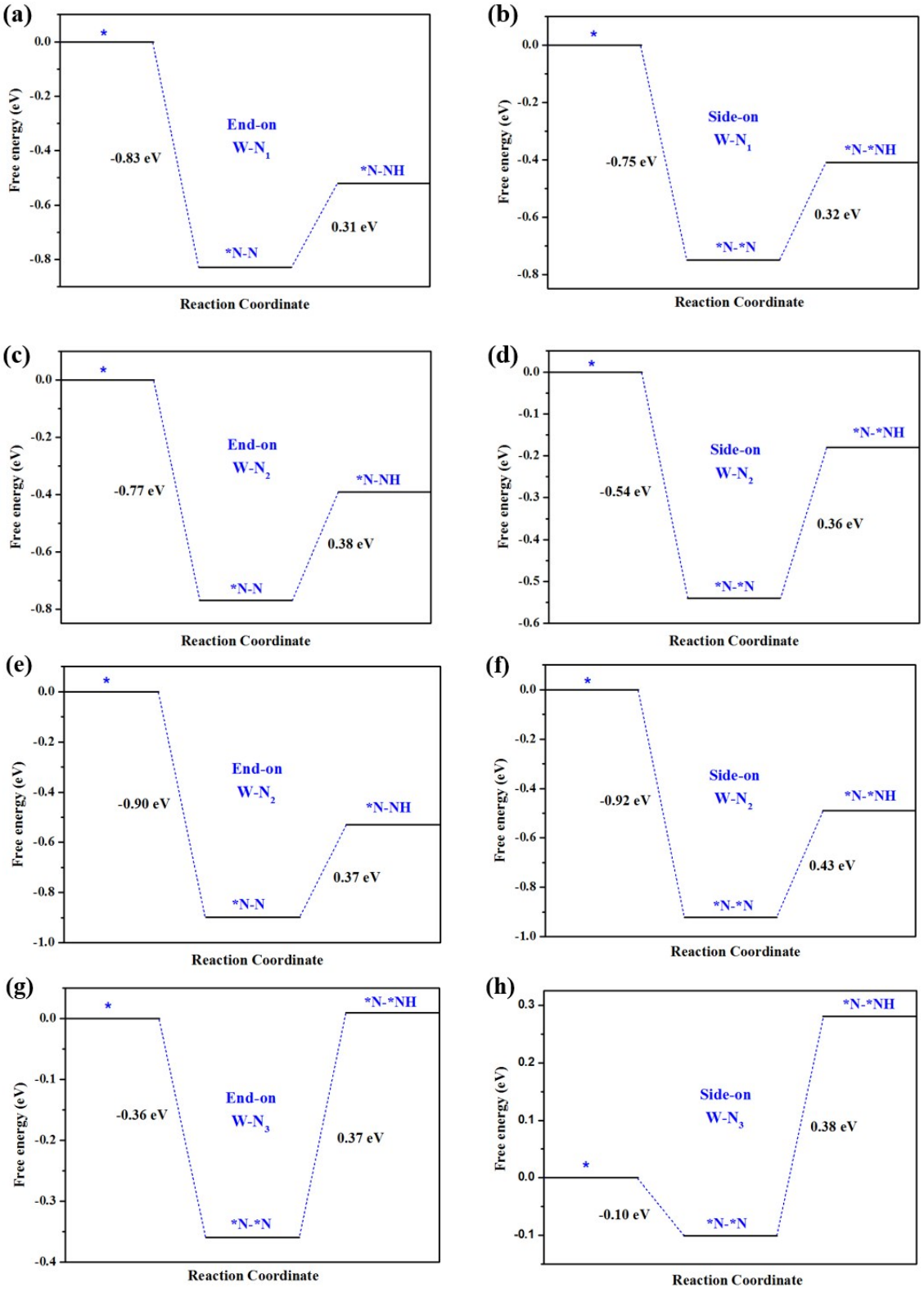

Figure S2. Calculated free energy diagrams for N_2 adsorption and protonation of end-on and side-on configurations for different N coordinates.

Table S1. The calculated zero point energies and entropy correction of different adsorption species, where the * represents the catalyst, *N≡*N and *N≡N refer to the side-on and end-on adsorption configurations, respectively.

Adsorption Species	E_{ZPE} (eV)	*-TS* (eV)
N_2	0.15	-0.58
*N≡*N	0.20	-0.19
*N=*NH	0.49	-0.13
*NH =*NH	0.77	-0.15
NH−NH_2	1.14	-0.17
NH_2−NH_2	1.48	-0.25
NH_2−NH_3	1.64	-0.29
N−NH_2	0.77	-0.12
*N	0.06	-0.04
*NH	0.34	-0.09
*NH_2	0.65	-0.14
*NH_3	1.03	-0.16
*N≡N	0.19	-0.18
*N=NH	0.45	-0.14
*NH=NH	0.81	-0.24
*NH−NH_2	1.11	-0.18
*NH_2−NH_2	1.42	-0.23
*N−NH_2	0.2	-0.18
NH_3	0.58	-0.56