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

Supporting Information

Single Transition Metal Atom Embedded into MoS_2 Nanosheet as a Promising Catalyst for Electrochemical Ammonia Synthesis

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Table S1. The charge transfer (ΔQ, $|e|$) and magnetic moment transfer ($\Delta\mu$, μ_B) between the adsorbed N_2 species and TM-doped MoS_2 monolayer.

TM	ΔQ	$\Delta\mu$
Sc	0.01	0.00
Ti	0.01	0.00
Cr	0.02	0.02
Mn	0.02	0.02
Rh	0.01	0.00
V	0.13	0.08
Fe	0.13	0.09
Co	0.11	0.08
Ni	0.10	0.07
Mo	0.08	0.06
Ru	0.09	0.06

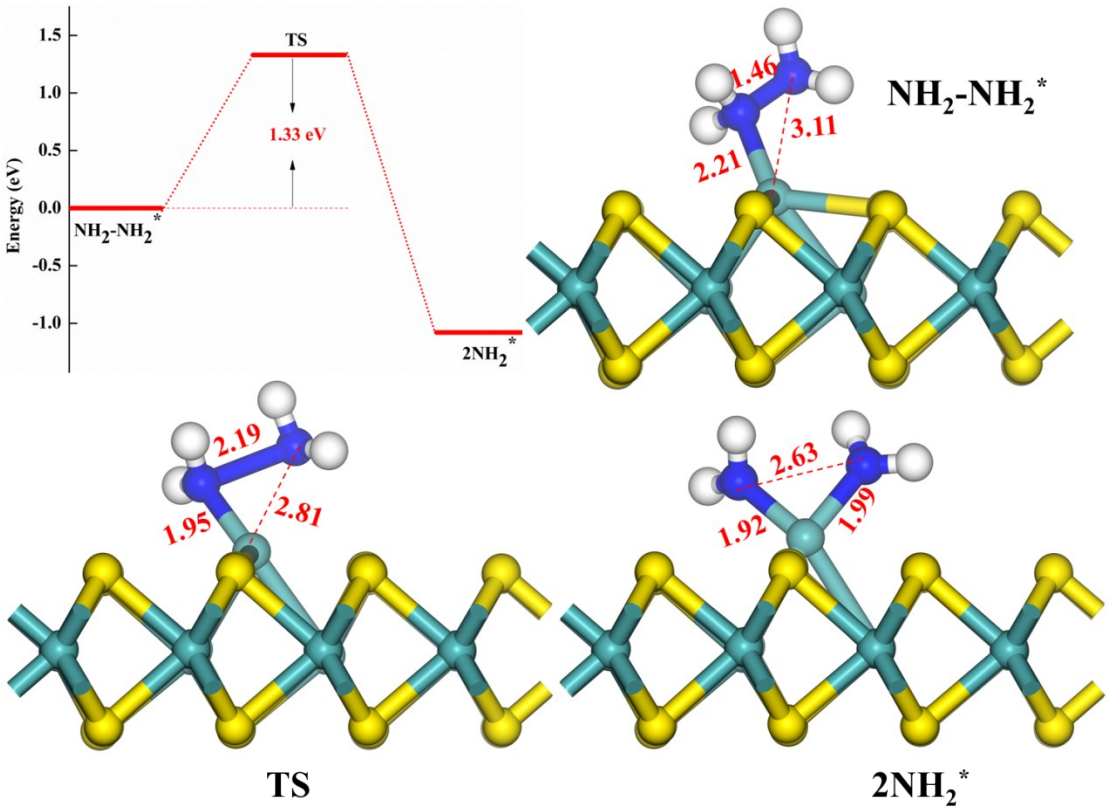

Fig. S1. The computed dissociation pathway of NH_2-NH_2^* to $2NH_2$ and the corresponding structures.

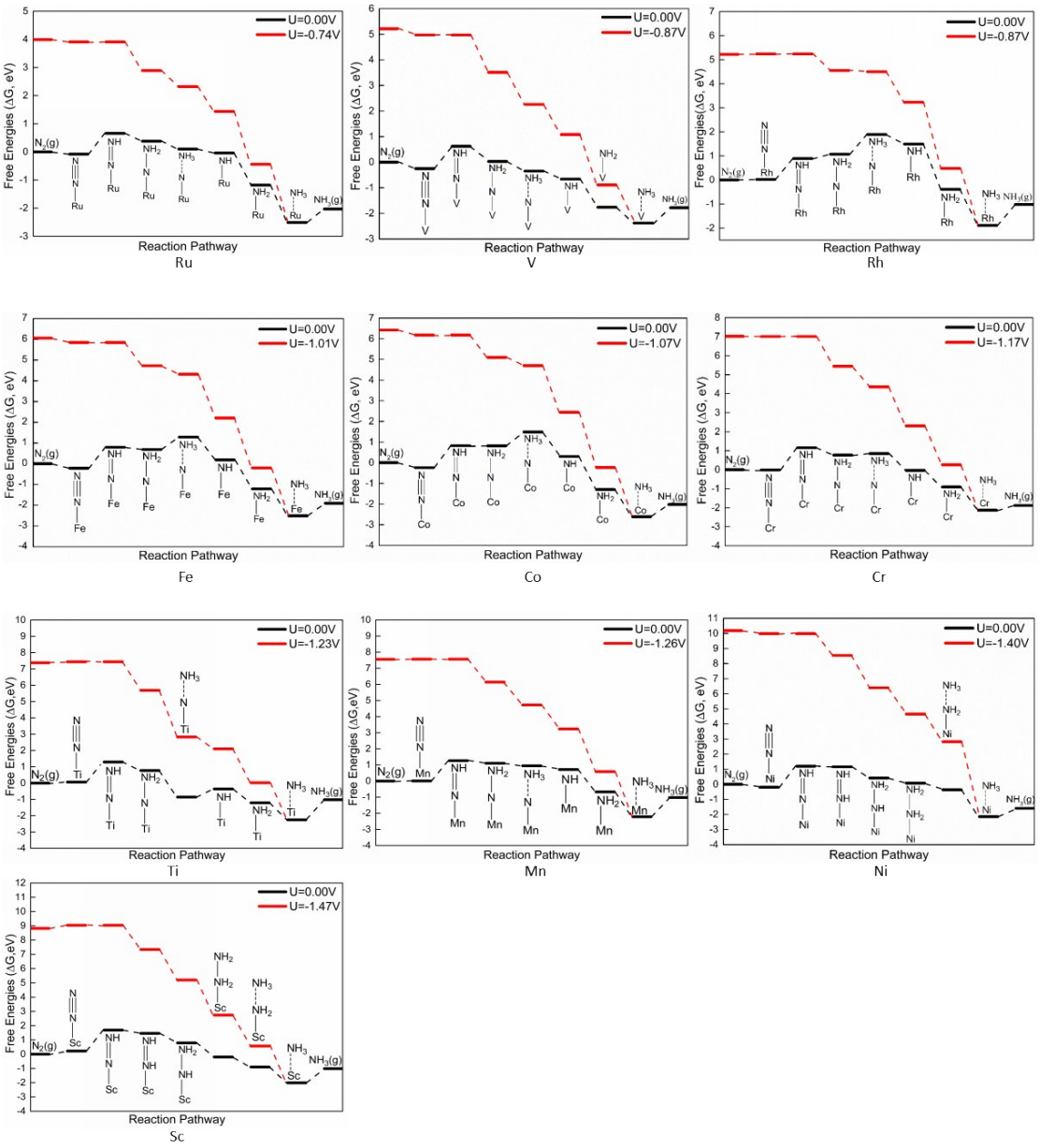

Fig. S2. The computed free energy profiles of NRR on various TM-doped MoS_2 nanosheets.