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

Nitrogen Fixation on defected Stanene Monolayer Embedded by single Mo atom: A Computational Study

Yao Tan, Ying Xu*

School of Physics and Electronic Science, Hunan University of Science and Technology, Xiangtan 411201, China

* Corresponding author,

Email address: yxu@hnust.edu.cn (Ying Xu)

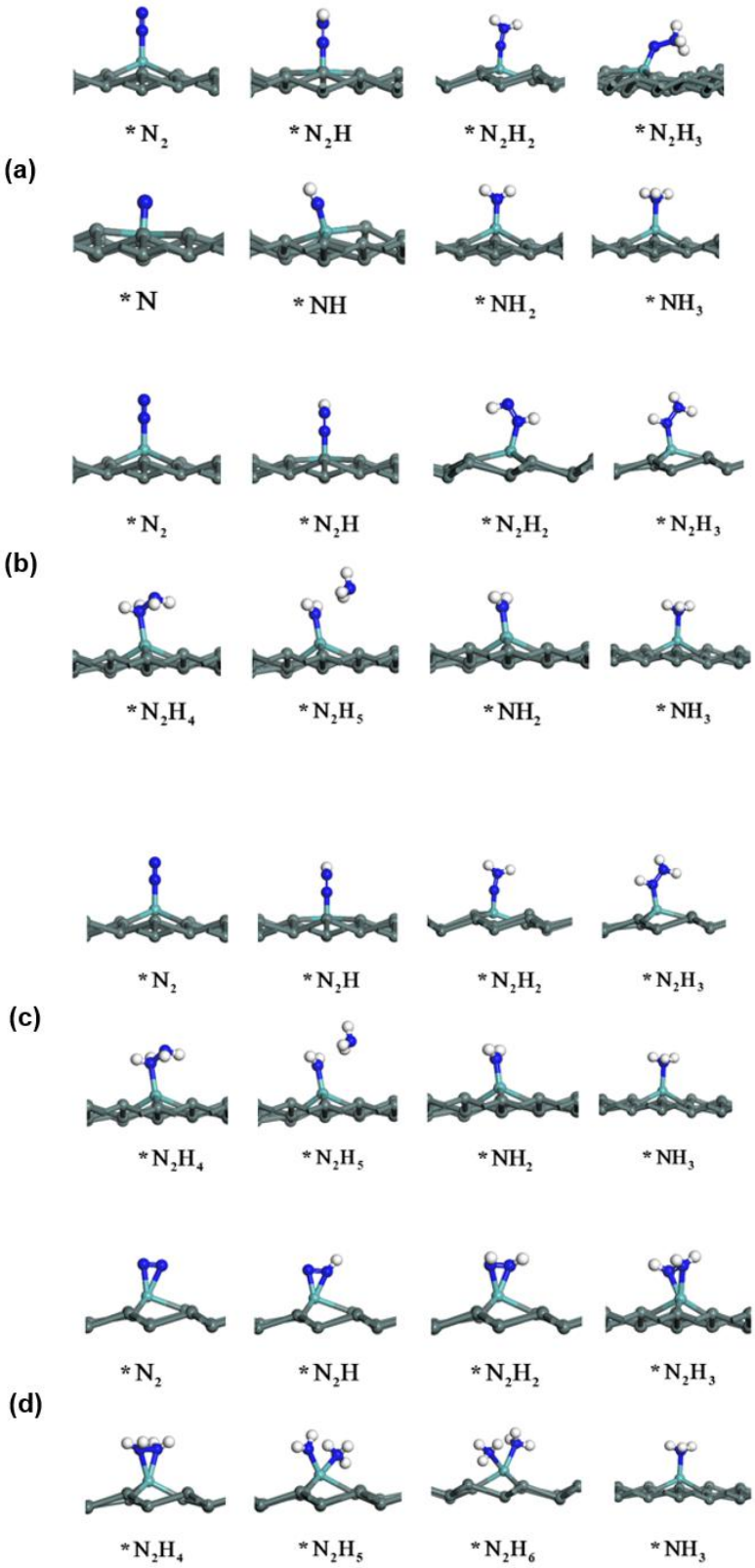

Figure S1. Optimized structures of the reaction intermediates through (a) distal, (b) alternating, (c) mixed, and (d) enzymatic pathways on the Mo/Stanene sheet.

.

Table S1. Calculated binding energies values of different transition metal atoms .

Transition metal atom	$Adsorption\ energy(eV)$
Ti	-4.57
V	-5.88
Fe	-3.67
Mn	-2.89
Ru	-6.58
Rh	-5.86
Co	-4.61
Ni	-5.04
Mo	-4.06

Table S2. Calculated ZPE and TS values of different species for end-on adsorption configuration, where the label * denotes the status of adsorption.

$Adsorbed\ species$	$E_{zpe}(eV)$	$TS(eV)$
N_2	0.15	0.59
$*N_2$	0.20	0.17
$*N$	0.08	0.07
$*NH$	0.35	0.10
$*NH_2$	0.64	0.15
$*NH_3$	1.02	0.16
$*NNH$	0.47	0.12
$*NNH_2$	0.80	0.20
$*NNH_3$	1.12	0.19
$*NHNH$	0.81	0.18
$*NHNH_2$	1.13	0.21
$*NH_2NH_2$	1.48	0.24
NH_3	0.91	0.60
H_2	0.27	0.40

Table S3. Calculated ZPE and TS values of different species for side-on adsorption configuration, where the label * denotes the status of adsorption.

$Adsorbed\ species$	$E_{zpe(eV)}$	$TS(eV)$
N_2	0.15	0.59
$*N_2$	0.18	0.16
$*N_2H$	0.47	0.15
$*N_2H_2$	0.78	0.17
$*N_2H_3$	1.15	0.18
$*N_2H_4$	1.47	0.24
$*N_2H_5$	1.68	0.26
$*N_2H_6$	2.03	0.31
$*NH_3$	1.02	0.16
NH_3	0.91	0.60
H_2	0.27	0.40