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Supplementary Information

First-principles screening of transition metal doped anatase TiO2(101) surfaces for the electrocatalytic nitrogen reduction

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Table S1, The Relative Energy of the Surface With the Dopant Doped at Different Sites(eV)

Dopants	Site1	Site2	Site3	Sit4
Ir	0	0.04642702	1.13668583	1.22735584
Cr	0	0.13701374	0.44476791	0.88816938
Sc	0	0.14180211	0.17622086	0.38880599
Mn	0	0.17880504	0.45128399	1.21131919
Fe	0	0.25752694	0.8250904	1.21900411
Rh	0	0.40830493	0.78291125	0.99736544
Pd	0	0.41392244	1.46027731	1.65723805
Au	0	0.64854325	1.00723349	1.29694066
Y	0	0.69018592	0.22867722	0.2516109
Pt	0	0.76974785	1.26679189	2.28242388
Ni	0	0.78979584	1.41399986	1.58480078
Zn	0	0.80827829	1.46800348	1.47259435
Cu	0	0.82690011	1.47392562	1.56611861
Co	0	0.89508919	1.34151027	1.52187035
Ag	0	0.92279324	1.78666584	1.44062722
Cd	0	1.1118456	1.36661965	1.35674563
Ru	0.03017855	0	0.62842579	0.7161452
Os	0.23726463	0	0.66701252	0.80772544
Re	0.79308001	0	0.19775126	0.29544987
V	0.07374279	0.09159066	0	0.07676651
Ta	1.7536626	0.44354855	0	0.01741497
Ti	7.32586921	0.44354855	0	0.01741497
Mo	0.60508138	0.5955415	0	0.01413072
Nb	1.36100314	0.92720478	0	0.01730005
W	1.53723415	1.22807506	0	0.05689599
Zr	0.81581405	0.64639455	0.01593083	0
Hf	0.93493218	0.59012864	0.0233688	0

Table S2, Formation Energy of the First ($E_f(O_v)$-1) and the Second ($E_f(O_v)$-2) O_v (eV)

dopant	$E_f(O_v)$-1	$E_f(O_v)$-2
Ag	-0.3359644	2.34642128
Au	0.65611048	2.7700783
Cd	-1.4097848	3.85951566
Co	1.28636153	3.59906865
Cr	2.68699097	
Cu	-0.4618405	3.58570648
Fe	2.38299295	3.57209457
Hf	3.62710024	
Ir	2.40863754	3.61604147
Mn	2.29503594	
Mo	3.43439207	
Nb	3.53690554	
Ni	0.52780412	3.61408031
Os	2.86180662	
Pd	0.73973172	3.57571971
Pt	1.3530939	3.57181038
Re	3.36616647	
Rh	1.91305502	3.61867798
Ru	2.93328707	
Sc	1.33138805	
Ta	3.56056076	
Ti	3.6	
V	3.53346483	
W	3.18229778	
Y	1.35973659	
Zn	-1.2839974	3.61478152
Zr	3.63499882	

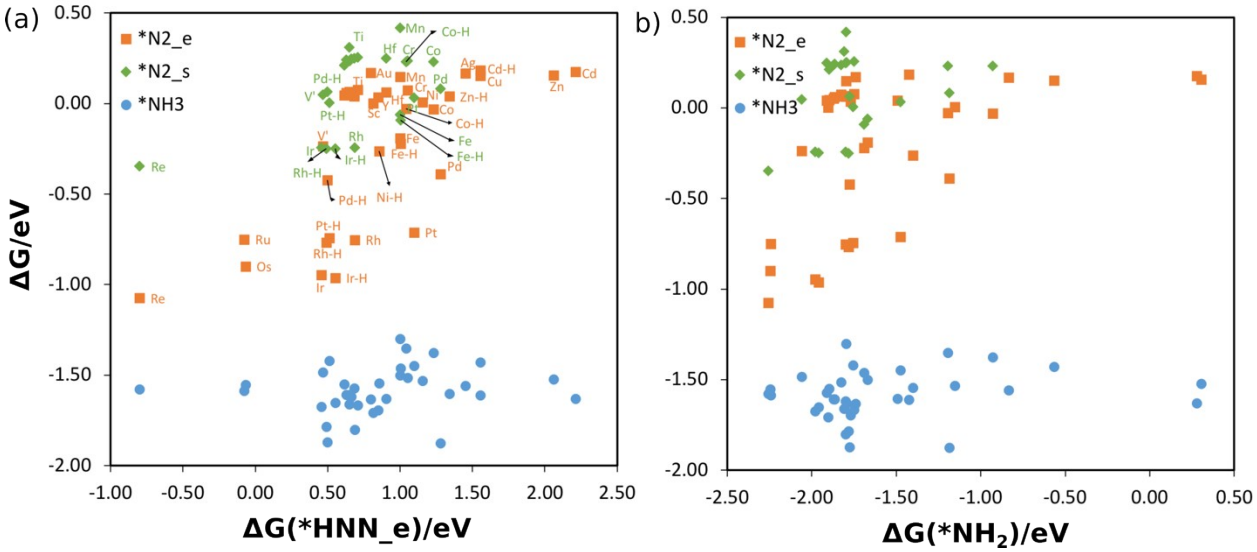

Figure S1, The scaling relation between the energy of $*N_2$_e, $*N_2$_s and $*NH_3$ against *HNN_e (a) and $*NH_2$(b).The data labeled as M-H presents the M-doped surface with an adsorbed H.

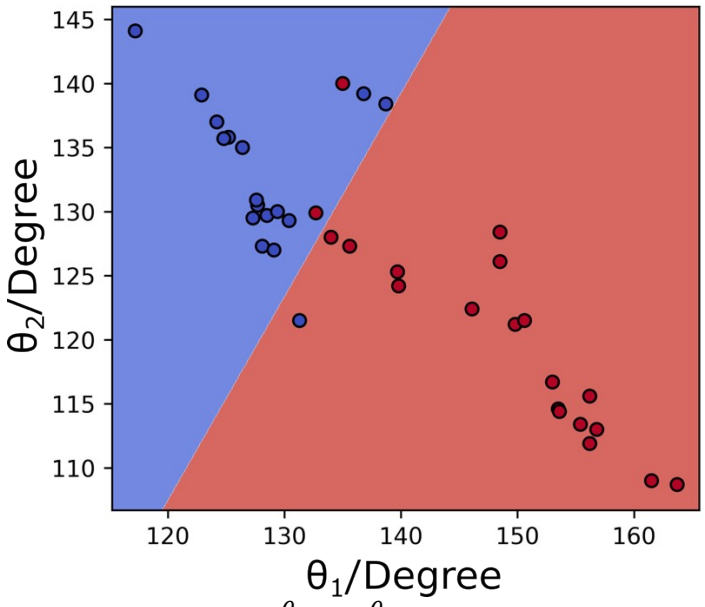

Figure S2, Classification of *HNN_e with θ_1 and θ_2 as features

Table S3, Accuracy of the SVM Algorithm for Classifying the Structure of *HNN

	Accuracy with different features				R^2	
	(L_1, L_2)	(θ_1, θ_2)	(L_1, L_2, θ_1)	$(L_1, L_2, \theta_1, \theta_2)$	Line 1	Line2
Re, Ru, Os to Group-I	84%	92%	100%	100%	0.79	0.98
Re, Ru, Os to Group-II	54%	86%	84%	89%	0.70	0.94

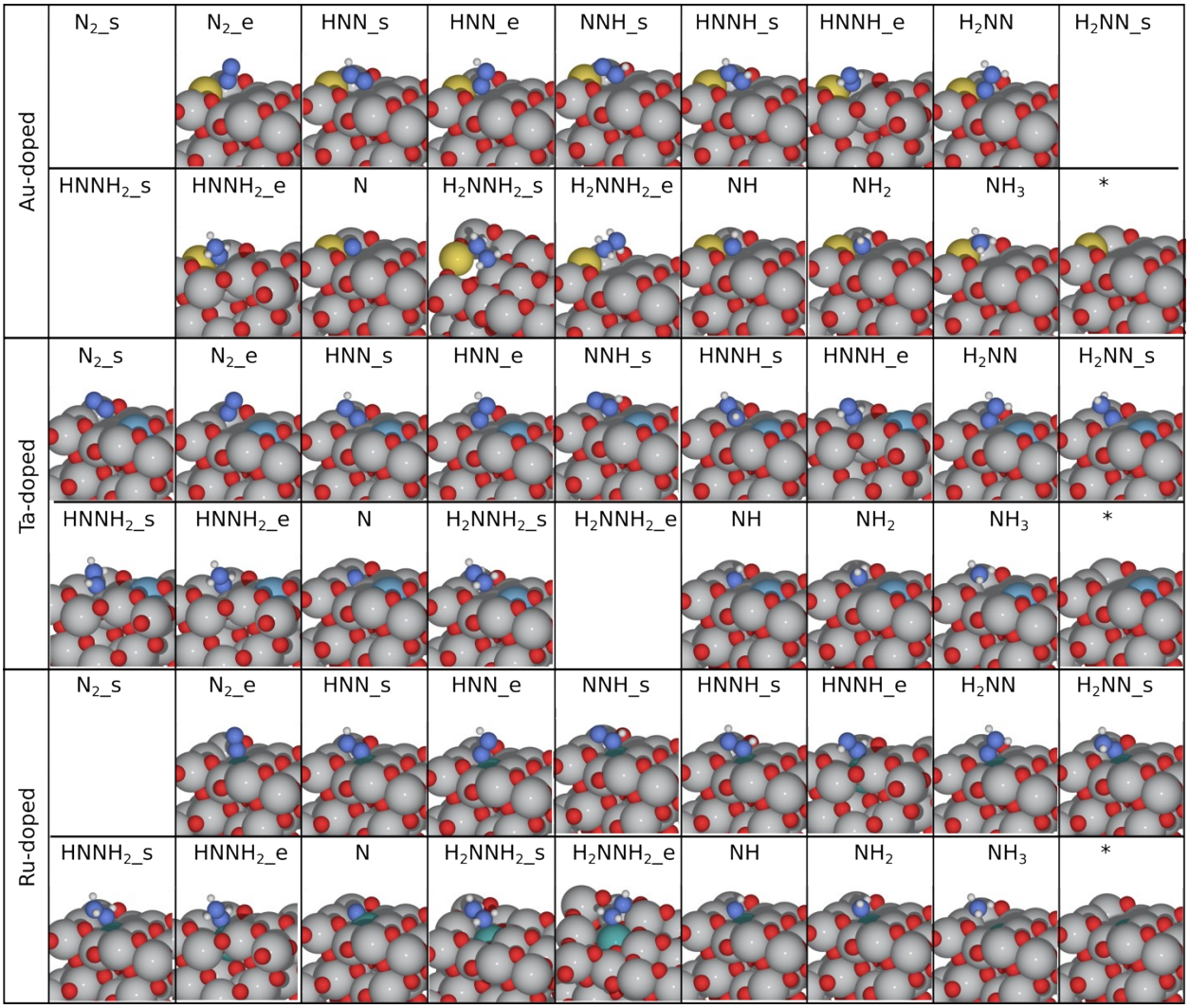

Figure S3, front view of all the optimized structures of the intermediates adsorbed on the Au, Ta, Ru-doped anatase TiO_2(101) surface.

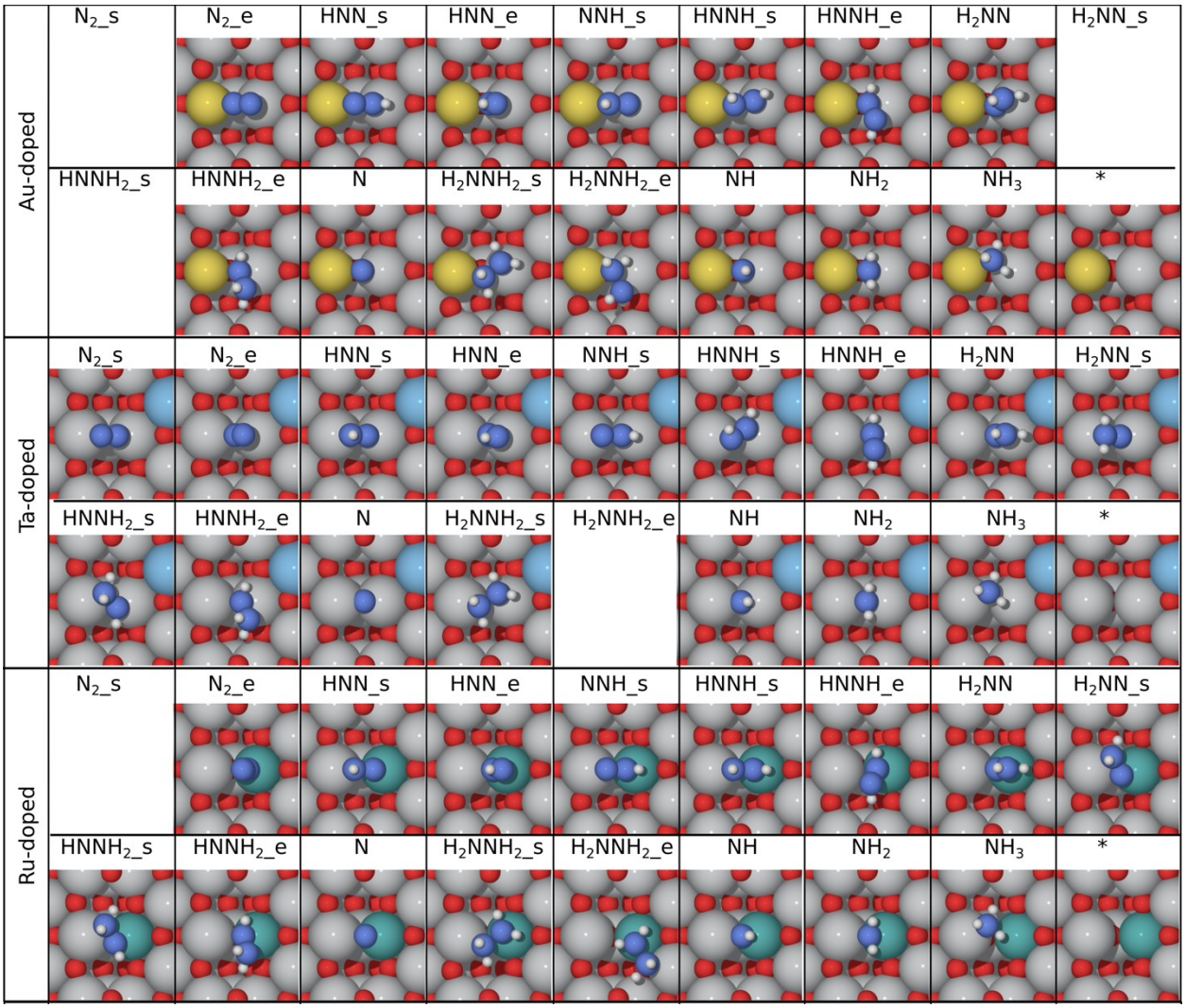

Figure S4, top view of all the optimized structures of the intermediates adsorbed on the Au, Ta, Ru-doped anatase TiO_2(101) surface.

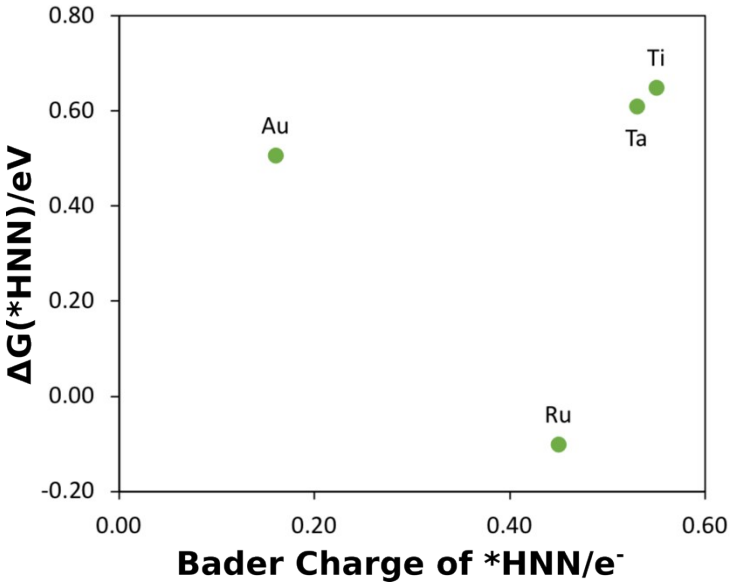

Figure S5, the energy of *HNN against its Bader Charge on the Au, Ta, Ru doped and the undoped anatase TiO_2(101) surface.