File description and total energies for DFT calculations

File name	Description	Total energy (eV)
n2	N_2 isolated molecule	-16.606
ni3x3	Ni (111) 3x3 supercell model surface	-234.228
n1-ni3x3	isolated N atom on Ni (111) 3x3 surface	-242.923
ts-diff-ni3x3	transition state for N diffusion on Ni (111)	-242.297
n+n-ni3x3	2 N_{ads} (adjacent) on Ni (111)	-251.110
ts-chemical-ni3x3	transition state for chemical step on Ni (111)	-249.471
n2-complex-ni3x3	$N_2^{\delta-}$ on Ni (111)	-250.904
n2-top-ni3x3	N_2 molecule adsorbed on Ni (111)	-251.482
ni6x3-step	Ni (111) monoatomic step 6x3 supercell model	-417.045
n1-step	isolated N atom on Ni (111) step	-426.033
ts-diff-step	transition state for N diffusion on Ni (111) step	-425.174
n+n-step	2 N_{ads} (adjacent) on Ni (111) step	-434.192
ts-chemical-step	transition state for chemical step on Ni (111) step	-433.132
n2-complex-step	$N_2^{\delta-}$ on Ni (111) step	-434.504
n2-ads-step	N_2 molecule adsorbed on Ni (111) step	-434.570
au11ni34	$Au_{11}Ni_{34}$ 3x3 supercell model surface (111) surface	-207.360
n1-au11ni34	isolated N atom on $Au_{11}Ni_{34}$	-214.673
ts-diff-au11ni34	transition state for N diffusion on $Au_{11}Ni_{34}$	-213.625
n+n-au11ni34	2 N_{ads} (adjacent) on $Au_{11}Ni_{34}$	-221.796
ts-chemical-au11ni34	transition state for chemical step on $Au_{11}Ni_{34}$	-221.114
n2-au11ni34	N_2 molecule adsorbed on $Au_{11}Ni_{34}$	-224.589