Supporting Information

Designing N, P-doped graphene surface-supported Mo single atom catalysts for efficient conversion of nitrogen into ammonia: A computational guideline

Ghada E. Khedr [a†], Samar M. Fawzy [b†], Icell M. Sharafeldin [b] and Nageh K. Allam [b*]

[a] *Department of Analysis & Evaluation, Egyptian Petroleum Research Institute (EPRI), Cairo 11727, Egypt.*

[b] *Energy Materials Laboratory, Physics Department, School of Sciences & Engineering, The American University in Cairo, New Cairo 11835, Egypt.*

**Corresponding Author's email: nageh.allam@aucegypt.edu*

† *Equal Contribution.*

Table S1. The dissolution potential (U_{diss}) of metal for the four catalysts

Structures	E_f (eV)	U_{diss} (eV)
MoP_4G	-2.76	0.57
MoN_1P_3G	-2.88	0.59
MoN_2P_2G α	-0.9	0.26
MoN_2P_2Gβ	-3.78	0.74
MoN_2P_2Gγ	-0.18	0.14
MoN_3P_1G	-4.8	0.91
MoN_4G	-4.32	0.83
MoG	-3.24	0.65

U_{diss} is calculated as $U_{diss} = U^0_{diss} - E_f/ne$, where U^0_{diss} and n represent the standard dissolution potential of bulk metal and the number of electrons included in the dissolution, respectively. E_f is calculated by $E_f = E_{Mo-P_nN_mG} - E_{P_nN_mG} - E_{Mo}$, where $E_{Mo\text{-}PnNmG}$, E_{PnNmG}, and E_{Mo} are the total energy of the catalyst, substrate, and molybdenum atom in its bulk structure, respectively.

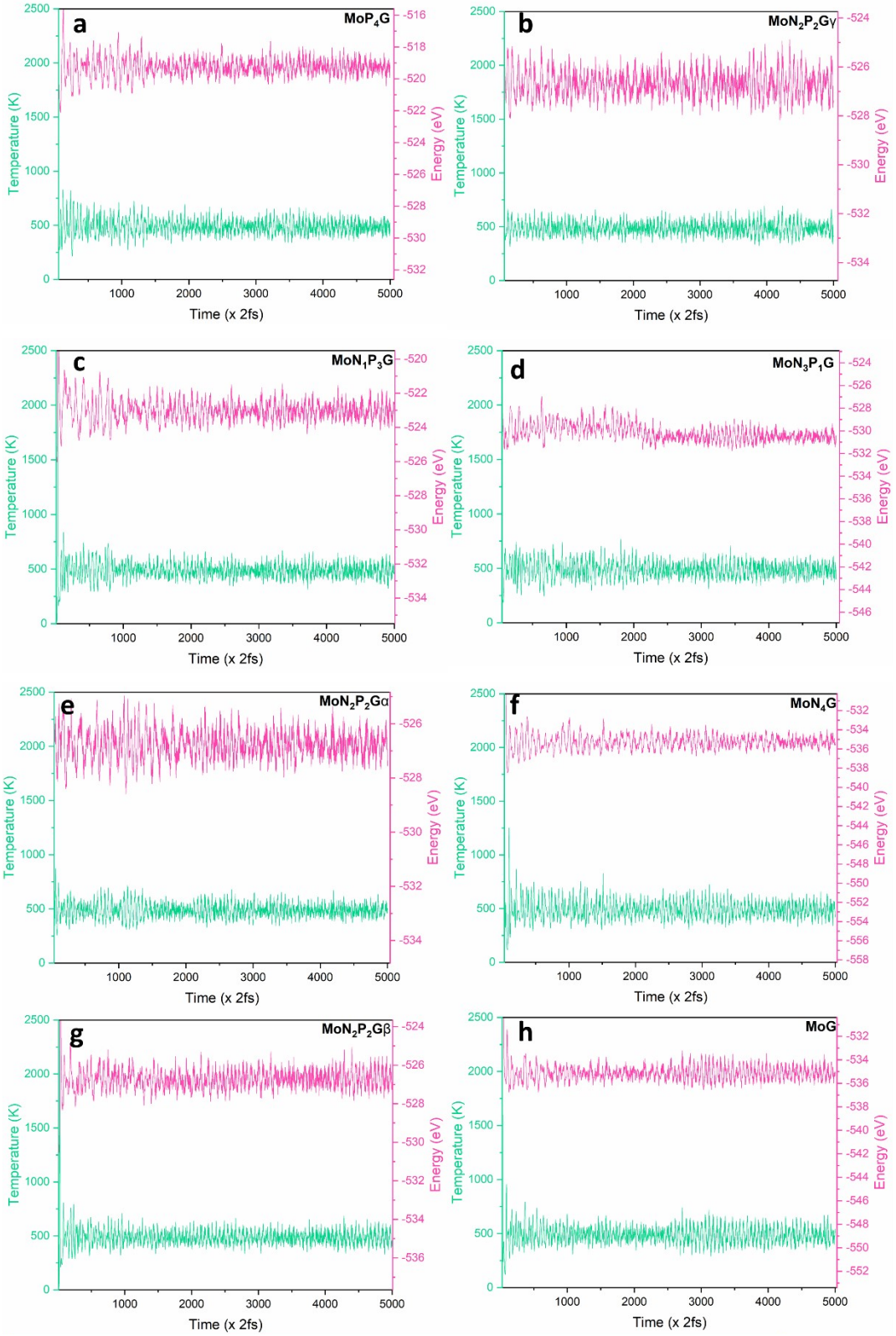

Figure S1. Total Energy and temperature variation with simulation time for the eight studied catalysts.