Supplementary information

Nitrogen Electroreduction and Hydrogen Evolution on Cubic Molybdenum Carbide: A Density Functional Study

Ivana Matanovic[a,b] and Fernando H. Garzon[*a,c]

[a] Chemical and Biological Engineering Department, Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM 87131, USA

[b] Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

[c] Sandia National Laboratory, Albuquerque, NM 87131, USA

*garzon@unm.edu

Table S1. Change in the free energies for the * + $1/2N_2$ → *N and *+ H^++e^-→*H reactions (in eV) on different cubic MoC and $MoC_{0.5}$ surfaces. * denotes a clean surface

MoC	[100]	[110]	(111)	(111)*	(311)	
Δ_rG (*+H^++e^-→*H)	0.61	-0.12	-0.40	-0.69	-0.45	
Δ_rG (*+$1/2N_2$ → *N)	-0.49	0.17	-1.20	-0.90	-0.38	
$MoC_{0.5}$	(001)	(100)/(010)	(101)	(111)	(111)*	(311)
Δ_rG (*+H^++e^-→*H)	0.48	-0.35	-0.39	-0.65	-0.59	-0.78
Δ_rG (*+ $1/2N_2$ → *N)	0.63	-0.08	-0.39	-2.09	-1.97	-1.89

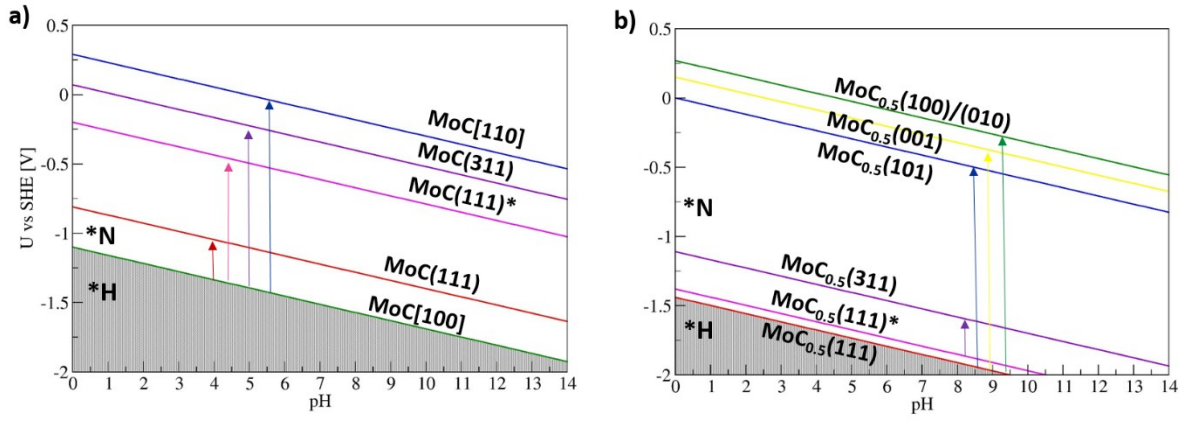

Figure S1. Pourbaix diagram of cubic a) MoC and b) $MoC_{0.5}$ that shows the conditions under which the surface will likely be covered with H-adatoms (grey) or N-adatoms (white). The Pourbaix diagrams were constructed using Δ_rG (*+H^++e^-→*H) and Δ_rG (*+$1/2N_2$ → *N) values from Table S1. The full lines show the conditions under which Δ_rG (*+H^++e^-→*H) = Δ_rG (*+$1/2N_2$ → *N). Vertical arrows show how the stability region of H-adatoms changes with the change of the surface structure.