

Electronic Supplementary Information

for

Nature of molybdenum carbide surfaces for catalytic hydrogen dissociation using machine-learned potentials: an ensemble-averaged perspective

¹

Woodrow N. Wilson,[†] John Michael Lane,[†] Chinmoy Saha,[†] Sony Severin,[†] Vivek S. Bharadwaj*,[‡] and Neeraj Rai*,[†]

[†]*Dave C. Swalm School of Chemical Engineering and Center for Advanced Vehicular Systems, Mississippi State University, Mississippi State, MS, 39762, USA*

[‡]*Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, CO, 80401, USA*

E-mail: neerajrai@che.msstate.edu

Phone: +1-662-325-0790. Fax: +1-662-325-2482

Table S1: Optimized Lattice Parameters for molybdenum and molybdenum carbides studied at the PBE+D3/DZVP-MOLOPT(SR)/600 Ry Level of Theory

		a	b	c	α	β	γ
Mo	Materials Project	3.17	3.17	3.17	90.00	90.00	90.00
	Calculated	3.09	3.09	3.09	90.00	90.00	90.00
	% Error	-2.52	-2.52	-2.52	0.00	0.00	0.00
α -Mo ₂ C	Materials Project	3.06	3.06	4.64	90.00	90.00	120.00
	Calculated	2.99	2.99	4.79	90.00	90.00	120.67
	% Error	-2.29	-2.29	3.23	0.00	0.00	0.56
β -Mo ₂ C	Materials Project	4.63	5.21	6.05	90.00	90.00	90.00
	Calculated	4.65	5.17	6.02	90.00	90.00	90.00
	% Error	0.43	-0.77	-0.50	0.00	0.00	0.00
δ -MoC	Materials Project	4.38	4.38	4.38	90.00	90.00	90.00
	Calculated	4.33	4.33	4.33	90.00	90.00	90.00
	% Error	-1.14	-1.14	-1.14	0.00	0.00	0.00

Table S2: Pressures (bar) estimated from the Ideal Gas Law

Surface	H ₂ Loading	Temperature (K)					
		450	525	600	750	825	900
$\alpha\text{-Mo}_2\text{C}$ (101)	25	0.00	0.00	0.00	1.18	4.76	17.79
	30	0.81	0.00	0.00	17.05	22.98	36.29
	90	196.69	252.59	306.03	401.08	453.15	512.83
$\beta\text{-Mo}_2\text{C}$ (001)	29	0.00	0.00	0.02	0.00	0.00	0.80
	34	0.00	0.00	0.00	0.04	0.32	0.11
	75	6.19	24.50	44.19	114.25	162.37	196.16
	107	64.11	139.68	225.60	350.64	431.59	520.16
$\delta\text{-MoC}$ (111)	23	3.97	14.55	11.97	28.83	37.41	31.07
	29	11.52	40.70	39.16	66.81	79.53	100.34
	53	75.59	163.67	175.90	267.21	343.94	351.11
	83	232.08	375.08	398.08	588.70	721.43	729.33
	124	535.48	767.37	802.04	1083.32	1277.36	1350.59
Mo (110)	25	0.00	0.00	0.00	0.00	0.13	0.00
	29	0.00	0.00	0.00	0.00	0.00	0.00
	61	2.78	3.42	2.01	6.69	14.19	36.84
	85	23.08	12.46	22.64	71.76	112.86	134.54

² Code Listing S1: CP2K

```
1 &FORCE_EVAL
2   METHOD Quickstep
3   STRESS_TENSOR ANALYTICAL
4   &DFT
5     BASIS_SET_FILE_NAME BASIS_MOLOPT
6     POTENTIAL_FILE_NAME POTENTIAL
7     UNRESTRICTED_KOHN_SHAM ON
8     &QS
9       EPS_DEFAULT 1.0E-10
10      EXTRAPOLATION USE_PREV_WF
11    &END
12    &SCF
13      EPS_SCF 1.0E-5
14      MAX_SCF 40
15      SCF_GUESS RESTART
16      &OUTER_SCF .TRUE.
17        EPS_SCF 1.0E-5
18        MAX_SCF 50
19      &END OUTER_SCF
20      &OT .TRUE.
21        ALGORITHM IRAC
22        MINIMIZER DIIS
23        N_HISTORY_VEC 7
24        PRECONDITIONER FULL_KINETIC
25        PRECOND_SOLVER INVERSE_CHOLESKY
26        ROTATION .TRUE.
27        OCCUPATION_PRECONDITIONER .TRUE.
28      &END OT
29    &END SCF
30    &XC
31      &XC_GRID
32        XC_DERIV NN10_SMOOTH
33        XC_SMOOTH_RHO NN10
34      &END XC_GRID
35      &VDW_POTENTIAL
36        POTENTIAL_TYPE PAIR_POTENTIAL
37        &PAIR_POTENTIAL
38          TYPE DFTD3(BJ)
39          REFERENCE_FUNCTIONAL PBE
40          R_CUTOFF 10.0
41          CALCULATE_C9_TERM .TRUE.
```

```

42          VERBOSE_OUTPUT .TRUE.
43          PARAMETER_FILE_NAME dftd3.dat
44      &END PAIR_POTENTIAL
45      &END VDW_POTENTIAL
46      &XC_FUNCTIONAL
47          &GGA_X_PBE
48          &END GGA_X_PBE
49          &GGA_C_PBE
50          &END GGA_C_PBE
51      &END XC_FUNCTIONAL
52  &END XC
53  &MGRID
54      CUTOFF 600
55      REL_CUTOFF 60
56      NGRIDS 5
57  &END MGRID
58  &LS_SCF
59      MAX_SCF 40
60  &END LS_SCF
61  &END DFT
62  &PRINT
63      &STRESS_TENSOR ON
64  &END STRESS_TENSOR
65  &END PRINT
66  &SUBSYS
67      &TOPOLOGY
68          CONN_FILE_FORMAT OFF
69          COORD_FILE_FORMAT XYZ
70          COORD_FILE_NAME start.xyz
71  &END TOPOLOGY
72  &CELL
73      PERIODIC XYZ
74      CELL_FILE_FORMAT CIF
75      CELL_FILE_NAME start.cif
76  &CELL_REF
77      PERIODIC XYZ
78      CELL_FILE_FORMAT CIF
79      CELL_FILE_NAME start.cif
80  &END CELL_REF
81  &END CELL
82  &KIND Mo
83      BASIS_SET DZVP-MOLOPT-SR-GTH
84      POTENTIAL GTH-PBE
85  &END KIND

```

```

86      &KIND O
87          BASIS_SET DZVP-MOLOPT-GTH
88          POTENTIAL GTH-PBE
89      &END KIND
90      &KIND H
91          BASIS_SET DZVP-MOLOPT-GTH
92          POTENTIAL GTH-PBE
93      &END KIND
94      &KIND C
95          BASIS_SET DZVP-MOLOPT-GTH
96          POTENTIAL GTH-PBE
97      &END KIND
98  &END SUBSYS
99  &END FORCE_EVAL
100 &MOTION
101   &GEO_OPT
102     TYPE MINIMIZATION
103     MAX_DR    1.0E-03
104     MAX_FORCE 1.0E-03
105     RMS_DR    1.0E-03
106     RMS_FORCE 1.0E-03
107     MAX_ITER 20
108     OPTIMIZER LBFGS
109   &LBFGS
110   &END
111   &END GEO_OPT
112   &MD
113     STEPS 20000
114     Timestep 0.5
115     ENSEMBLE NVT
116     TEMPERATURE 1000
117   &THERMOSTAT
118     REGION GLOBAL
119     TYPE NOSE
120     &NOSE
121       TIMECON [fs] 50.0
122     &END
123   &END THERMOSTAT
124   &BAROSTAT
125     PRESSURE [bar] 20.0
126     TIMECON [fs] 100.0
127     VIRIAL XYZ
128   &END
129   &END

```

```
130    &PRINT
131        &VELOCITIES
132        &END
133        &STRESS
134        &END
135        &FORCES
136        &END
137        &CELL
138        &END
139        &END
140    &END
141
142    &GLOBAL
143        PROJECT cp2k-md
144        PRINT_LEVEL LOW
145        RUN_TYPE MD
146    &END GLOBAL
147
```

³ Code Listing S2: MACE

```
1 #!/bin/bash
2
3 export CUDA_VISIBLE_DEVICES=0
4 #export CUDA_VISIBLE_DEVICES=0,1,2,3
5 for sd in 314 42 914;
6     do
7         nlayers=2
8         rc=5
9         lmax=1
10        body_order=2
11        nfeat=128
12        device=cuda # cpu or cuda
13        nepoch=50
14        nsawa=35
15
16        mace_run_train \
17            --name="mace-$sd" \
18            --train_file="train.xyz" \
19            --valid_fraction=0.05 \
20            --test_file="test.xyz" \
21            --E0s="isolated" \
22            --energy_key="energy" \
23            --forces_key="forces" \
24            --stress_key="stress" \
25            --compute_stress=True \
26            --model="MACE" \
27            --num_interactions=$nlayers \
28            --num_channels=$nfeat \
29            --max_L=$lmax \
30            --correlation=$body_order \
31            --forces_weight=1000 \
32            --energy_weight=10 \
33            --r_max=$rc \
34            --batch_size=5 \
35            --valid_batch_size=5 \
36            --max_num_epochs=$nepoch \
37            --start_swa=$nsawa \
38            --scheduler_patience=5 \
39            --patience=15 \
40            --eval_interval=1 \
41            --ema \
```

```
42      --swa \
43      --swa_forces_weight=10 \
44      --error_table="PerAtomRMSE" \
45      --default_dtype="float32" \
46      --device=$device \
47      --seed=$sd \
48      --restart_latest \
49      --save_cpu > /dev/null 2> /dev/null &
50
51      export CUDA_VISIBLE_DEVICES=$((CUDA_VISIBLE_DEVICES + 1 ))
52
53 done
54 wait
```

4 Code Listing S3: Source code for adding a ghost atom grid
5 to a training set

```
1 import os
2 import numpy as np
3 from ase import Atoms
4 from ase.io import iread, write
5 from ase.constraints import FixAtoms
6
7 ##### Inputs #####
8
9 traj_file = "db.xyz"
10 outfile = "db_grid.xyz"
11 ghost_element = "Fr"
12 rcut = 5.0
13
14 ##### CODE STARTS HERE #####
15 try:
16     os.remove(outfile)
17 except OSError:
18     pass
19
20 traj = iread(traj_file)
21
22 for atoms in traj:
23     cell = atoms.get_cell()
24     hmat = cell.T
25     grid_resolution = np.zeros(3, dtype = int)
26     for idx, latvec in enumerate(cell):
27         length = np.linalg.norm(latvec)
28         ngrid_points = np.ceil(length / rcut)
29         grid_resolution[idx] = ngrid_points
30
31     sx = np.linspace(0, 1, grid_resolution[0], endpoint = False)
32     sy = np.linspace(0, 1, grid_resolution[1], endpoint = False)
33     sz = np.linspace(0, 1, grid_resolution[2], endpoint = False)
34
35     scaled_positions = np.vstack(np.meshgrid(sx,sy,sz)).reshape(3,-1).T
36     positions = (hmat @ scaled_positions.T).T
37
38     grid_atoms = Atoms(ghost_element * len(positions), positions)
39     ngrid_atoms = len(grid_atoms)
```

```
40
41     atoms += grid_atoms
42
43     c = FixAtoms(indices=[atom.index for atom in atoms if atom.symbol == ghost_element])
44     atoms.set_constraint(c)
45
46     write(outfile, atoms, append=True)
```

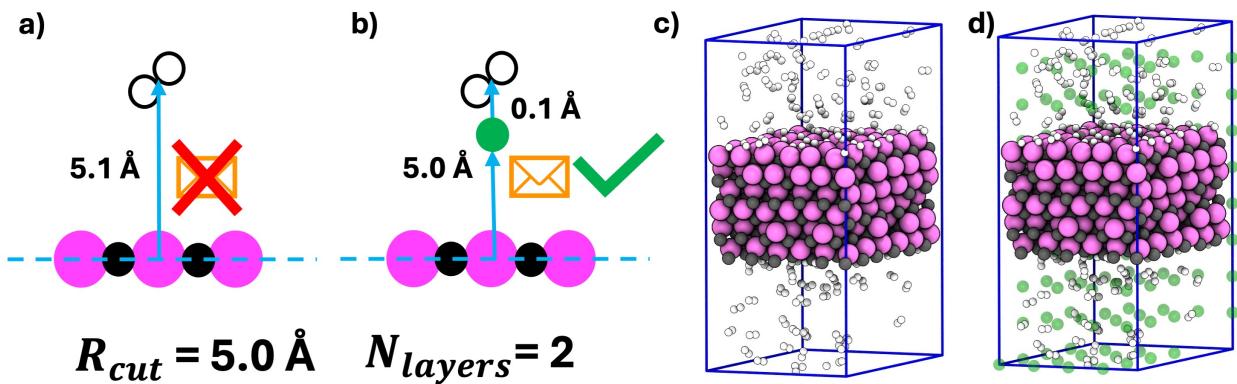


Figure S1: Illustration of the atoms being outside the cutoff radius of the message passing neural network (a), how the message passing can pass to atoms outside of the cutoff radius through an extra grid point (b), δ-MoC with 124 H₂ molecules with the ghost atom grid hidden (c), the same system and simulation snapshot showing the grid (d)

6 Code Listing S4: Python script for running MD with a
7 ghost atom grid

```
1 import numpy as np
2 from ase.io import read
3 from ase import Atoms, units
4 from ase.md.langevin import Langevin
5 from ase.md.velocitydistribution import (
6     Stationary,
7     ZeroRotation,
8     MaxwellBoltzmannDistribution,
9 )
10 from ase.constraints import FixAtoms
11 from mace.calculators import MACECalculator
12
13
14 def main():
15
16     ##### Inputs #####
17     # init_config must also contain lattice vectors, PBC, etc...
18     init_config = "start.xyz"
19     seed = 42
20     temperature = 900
21     nsteps = 1000000
22     dt = 0.5
23     restart = False
24
25     using_ghost_grid = True
26     ghost_element = "Fr"
27     gres = 5.0
28
29     freq = 20
30     logfile = "langevin.log"
31     trajfile = "langevin.traj"
32
33     # Define the potential energy surface
34     calc = MACECalculator(
35         model_paths=["model_swa.model"],
36         device="cuda",
37         default_dtype="float32",
38     )
39
```

```

40 ##### Code starts here #####
41 np.random.seed(seed)
42 atoms = read(init_config)
43 atoms.calc = calc
44
45 if using_ghost_grid:
46     apply_ghost_grid(atoms, ghost_element, gres)
47
48 run_MD(atoms, dt, temperature, trajfile, logfile, nsteps, freq, restart)
49
50
51 def apply_ghost_grid(atoms, ghost_element="Fr", rcut=5.0):
52     cell = atoms.get_cell()
53     hmat = cell.T
54     grid_resolution = np.zeros(3, dtype=int)
55     for idx, latvec in enumerate(cell):
56         length = np.linalg.norm(latvec)
57         ngrid_points = np.ceil(length / rcut)
58         grid_resolution[idx] = ngrid_points
59
60     sx = np.linspace(0, 1, grid_resolution[0], endpoint=False)
61     sy = np.linspace(0, 1, grid_resolution[1], endpoint=False)
62     sz = np.linspace(0, 1, grid_resolution[2], endpoint=False)
63
64     scaled_positions = np.vstack(np.meshgrid(sx, sy, sz)).reshape(3, -1).T
65     positions = (hmat @ scaled_positions.T).T
66
67     grid_atoms = Atoms(ghost_element * len(positions), positions)
68     ngrid_atoms = len(grid_atoms)
69
70     atoms += grid_atoms
71
72     c = FixAtoms(indices=[atom.index for atom in atoms if atom.symbol == ghost_element])
73     atoms.set_constraint(c)
74
75
76 def run_MD(atoms, dt, temperature, trajfile, logfile, nsteps, freq, restart=False):
77     if restart:
78         dyn = Langevin(
79             atoms,
80             dt * units.fs,
81             temperature_K=temperature,
82             friction=0.01 / units.fs,
83             logfile=logfile,

```

```

84         trajectory=trajfile,
85         loginterval=freq,
86         append_trajectory=True,
87     )
88     traj = Trajectory(trajfile)
89     last_config = traj[-1]
90     atoms.set_positions(last_config.get_positions())
91     atoms.set_momenta(last_config.get_momenta())
92     dyn.nsteps = (len(traj) - 1) * freq
93
94 else:
95     dyn = Langevin(
96         atoms,
97         dt * units.fs,
98         temperature_K=temperature,
99         friction=0.01 / units.fs,
100        logfile=logfile,
101        trajectory=trajfile,
102        loginterval=freq,
103    )
104    MaxwellBoltzmannDistribution(atoms, temperature_K=temperature)
105    Stationary(atoms)
106    ZeroRotation(atoms)
107
108    dyn.run(nsteps)
109
110
111 if __name__ == "__main__":
112     main()

```

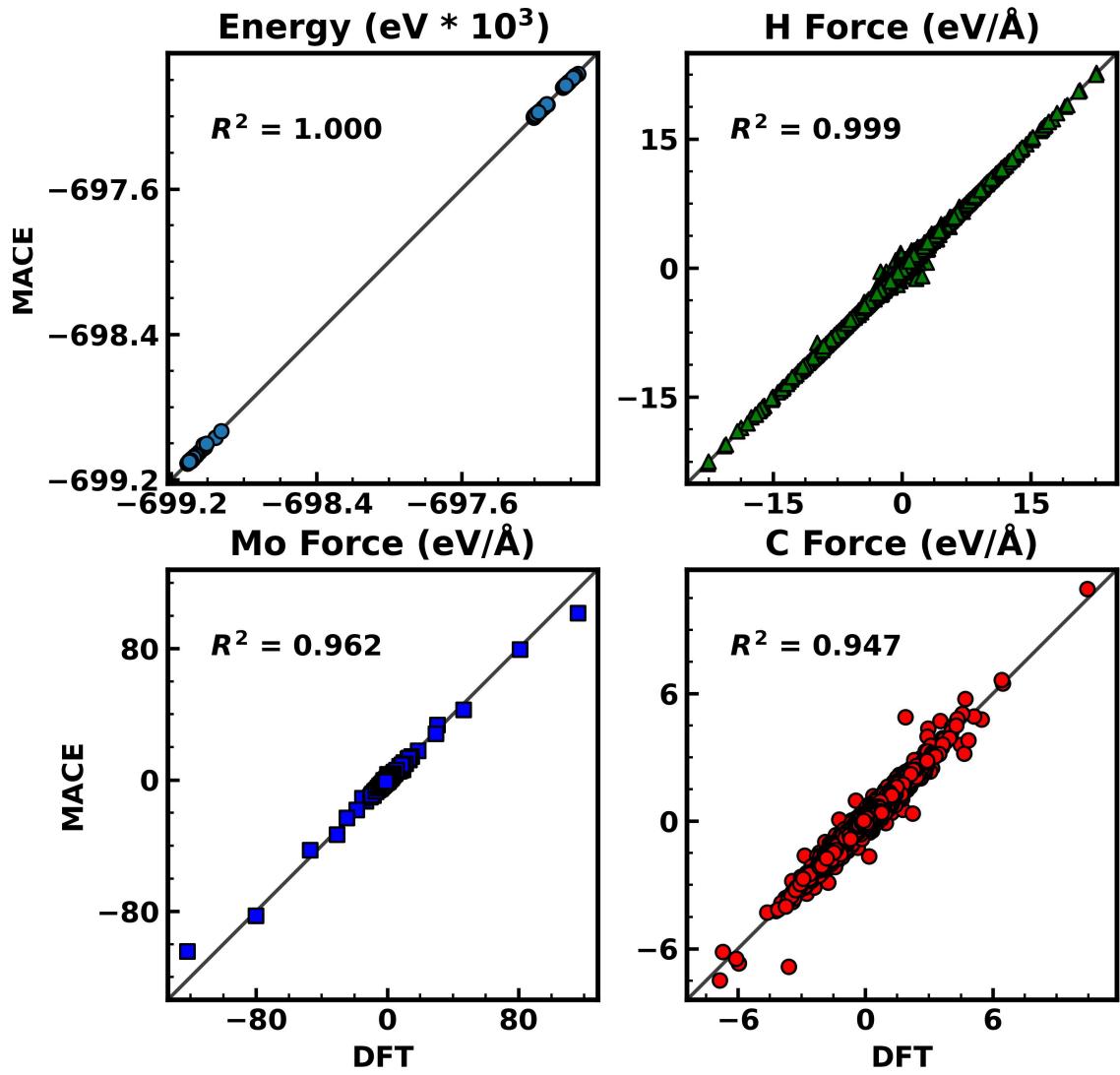


Figure S2: Energy and force parity plots with trained MACE model on test data for α -Mo₂C

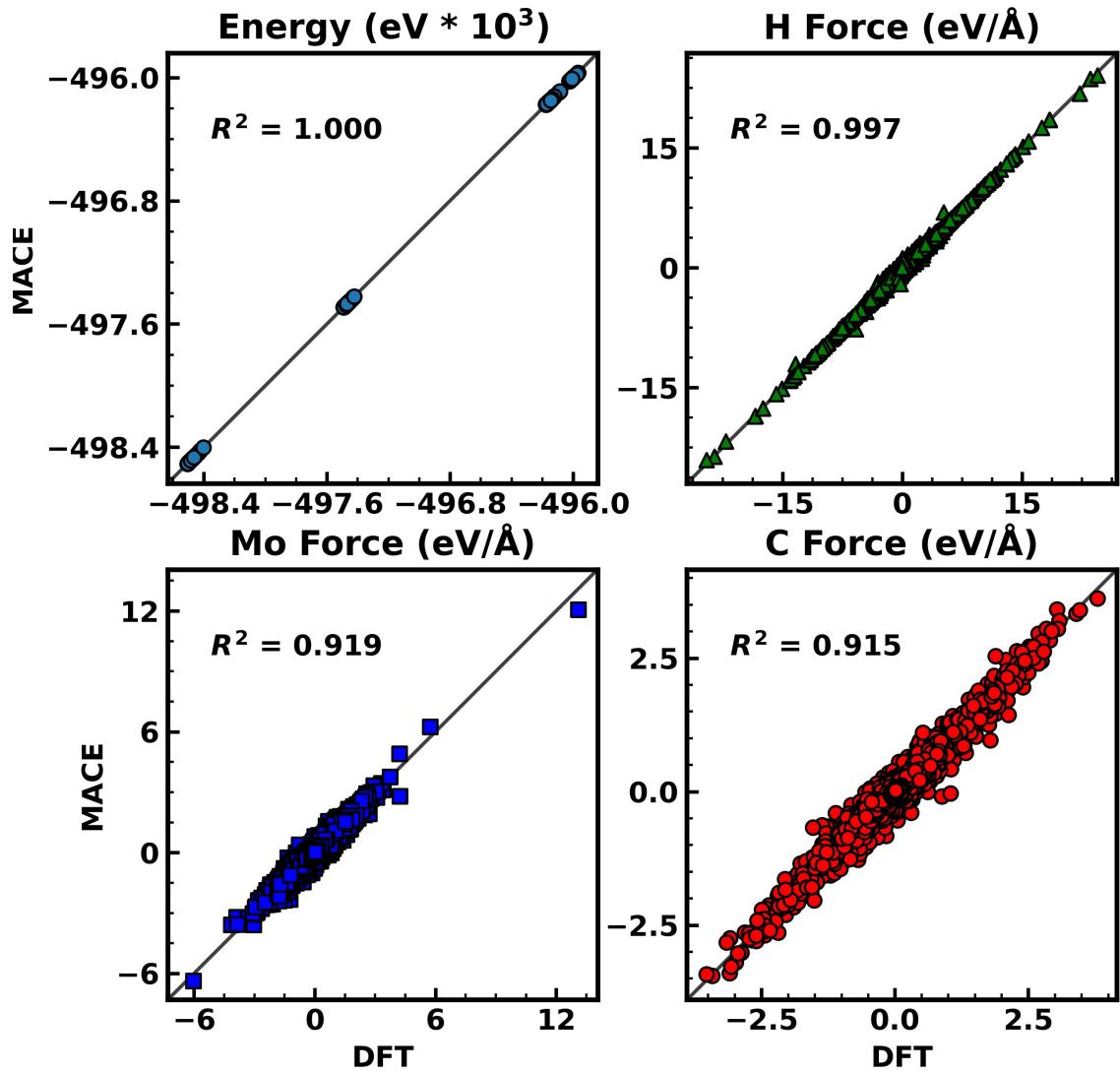


Figure S3: Energy and force parity plots with trained MACE model on test data for β -Mo₂C

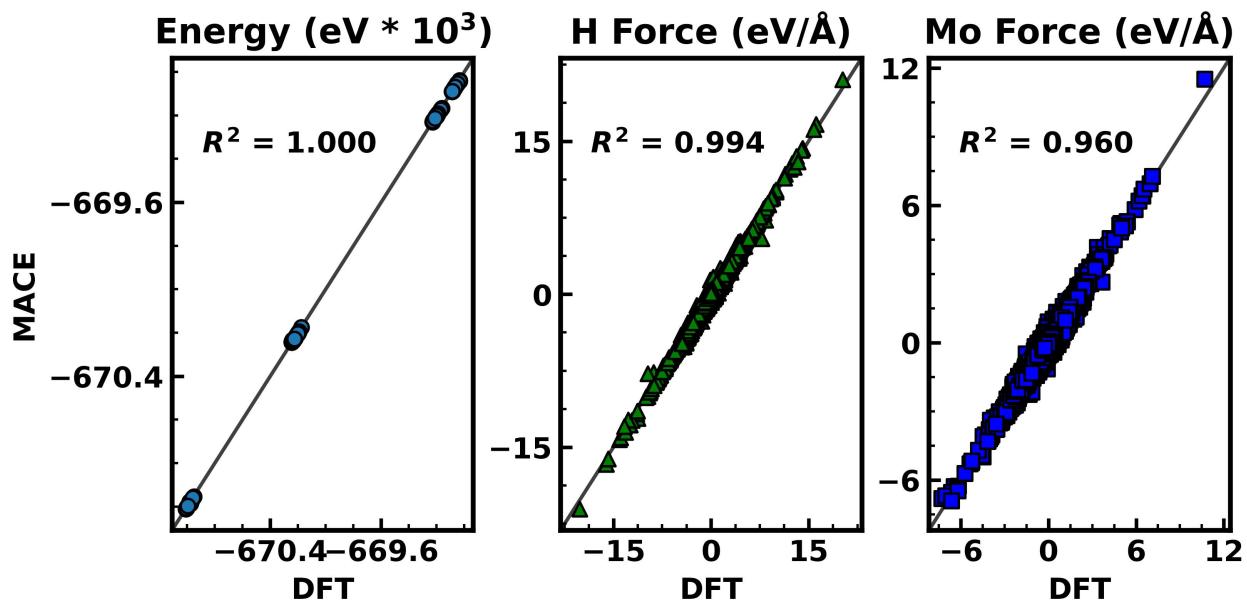


Figure S4: Energy and force parity plots with trained MACE model on test data for Mo

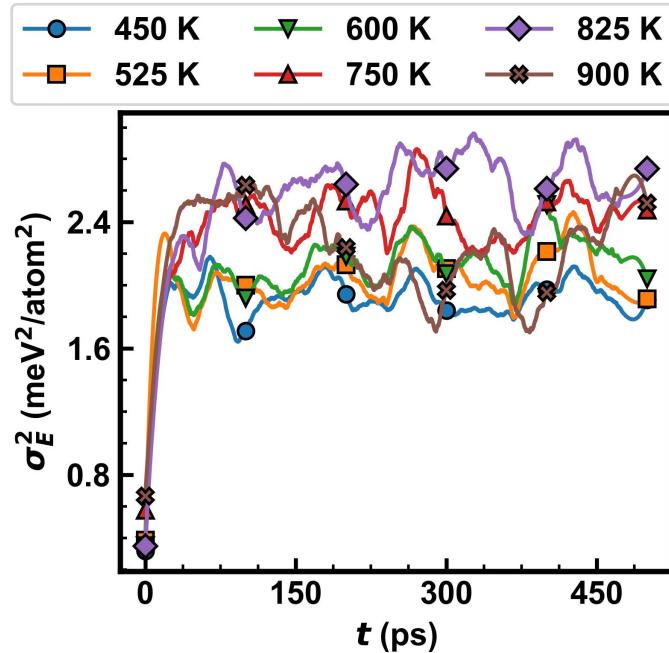


Figure S5: Post processing active learning on a MD trajectory of 25 H₂ molecules over α -Mo₂C

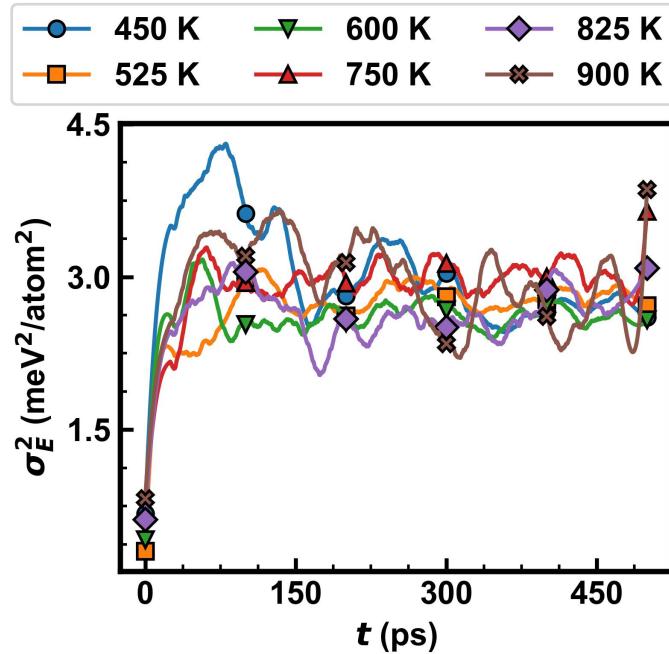


Figure S6: Post processing active learning on a MD trajectory of 30 H₂ molecules over α -Mo₂C

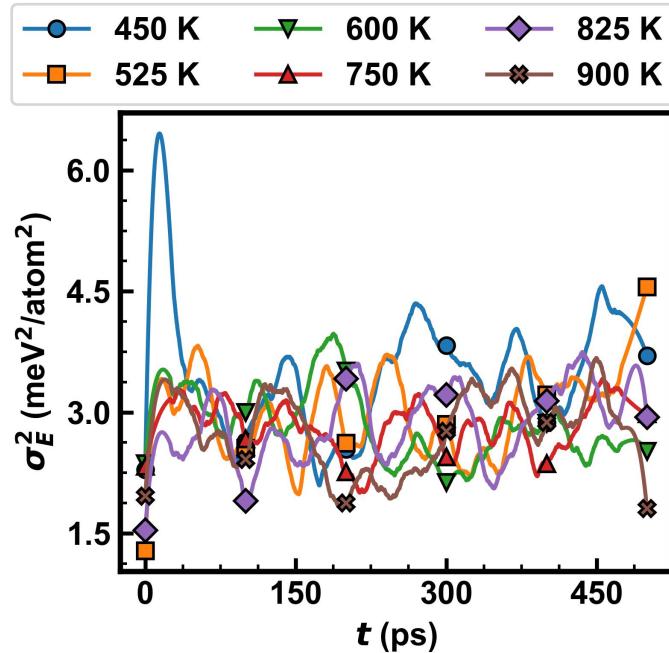


Figure S7: Post processing active learning on a MD trajectory of 90 H₂ molecules over α -Mo₂C

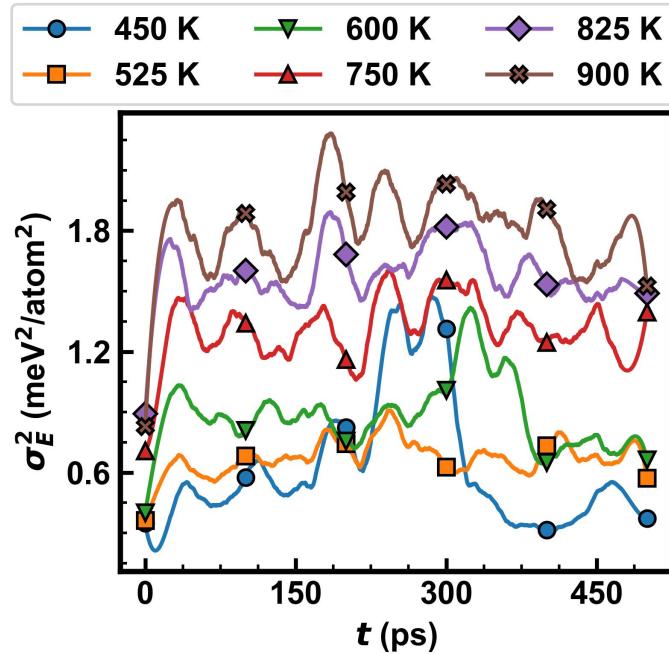


Figure S8: Post processing active learning on a MD trajectory of 29 H₂ molecules over β -Mo₂C

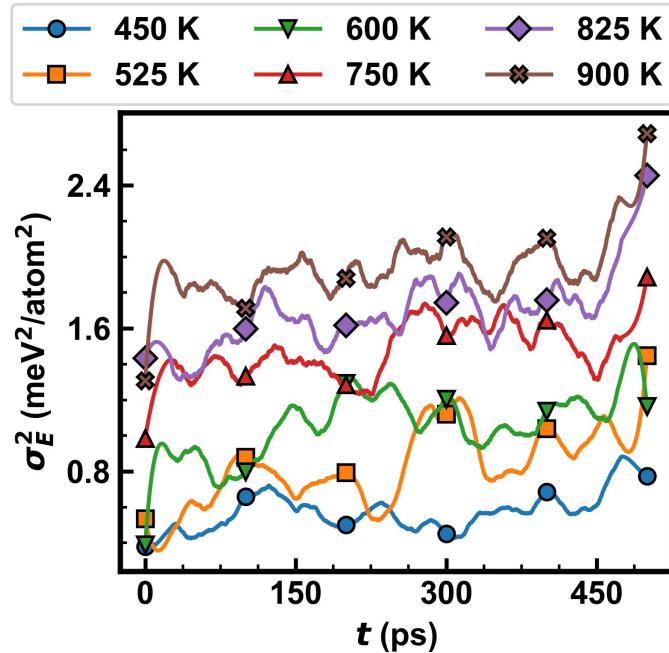


Figure S9: Post processing active learning on a MD trajectory of 34 H₂ molecules over β -Mo₂C

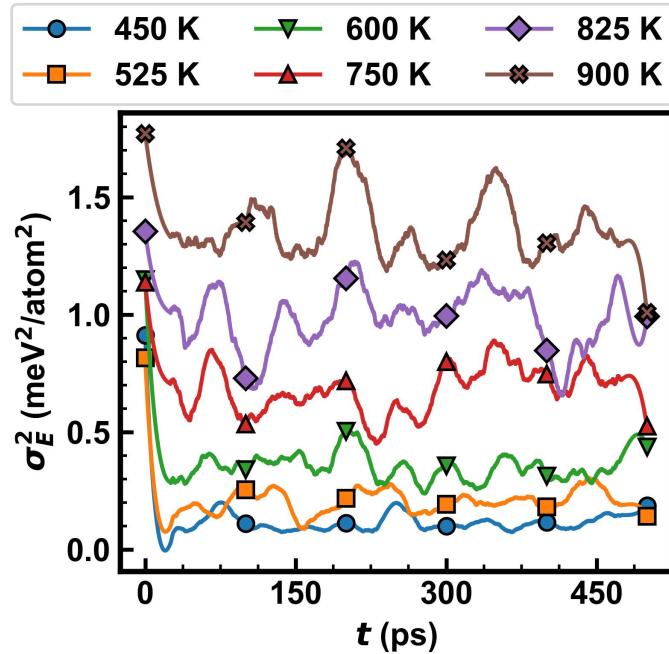


Figure S10: Post processing active learning on a MD trajectory of 75 H₂ molecules over β -Mo₂C

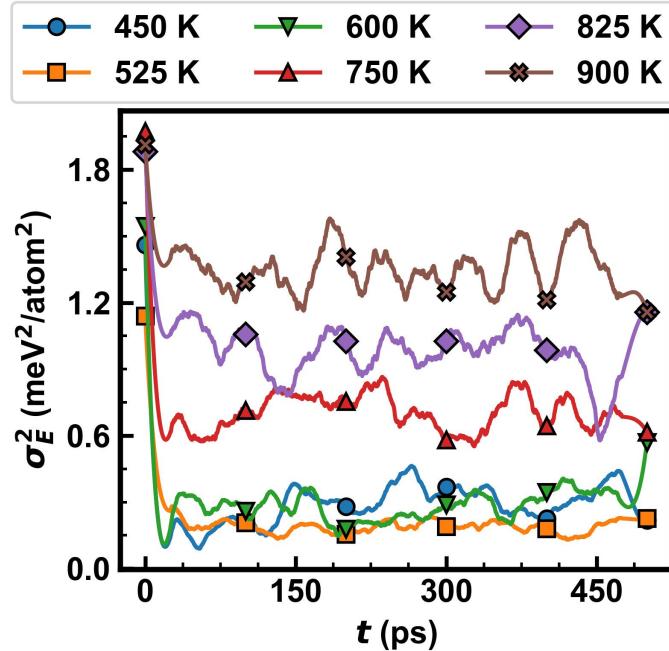


Figure S11: Post processing active learning on a MD trajectory of 107 H₂ molecules over β -Mo₂C

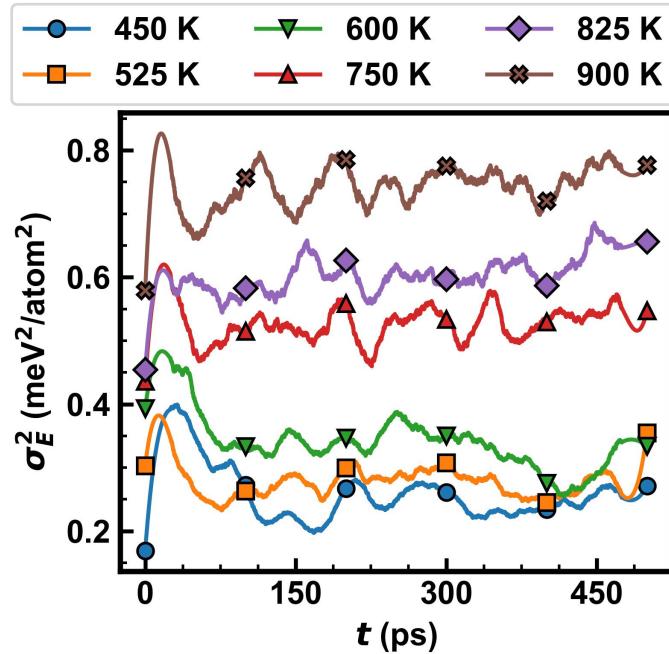


Figure S12: Post processing active learning on a MD trajectory of 23 H₂ molecules over δ -MoC

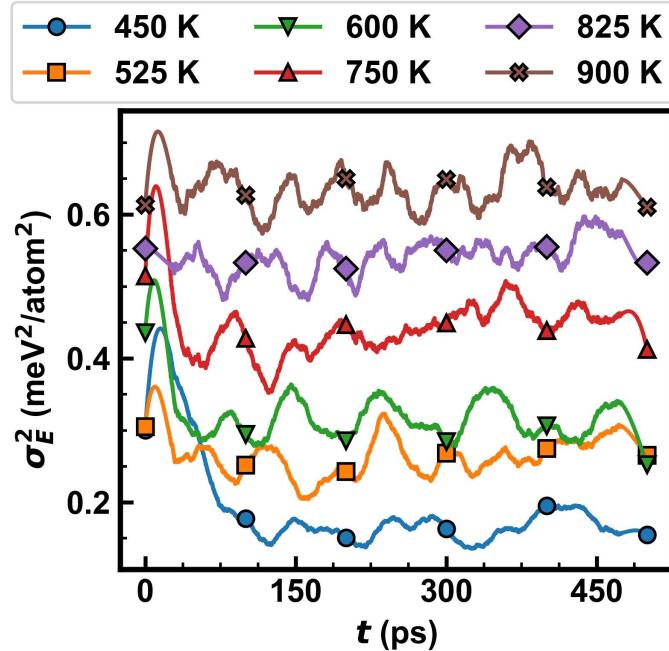


Figure S13: Post processing active learning on a MD trajectory of 29 H₂ molecules over δ-MoC

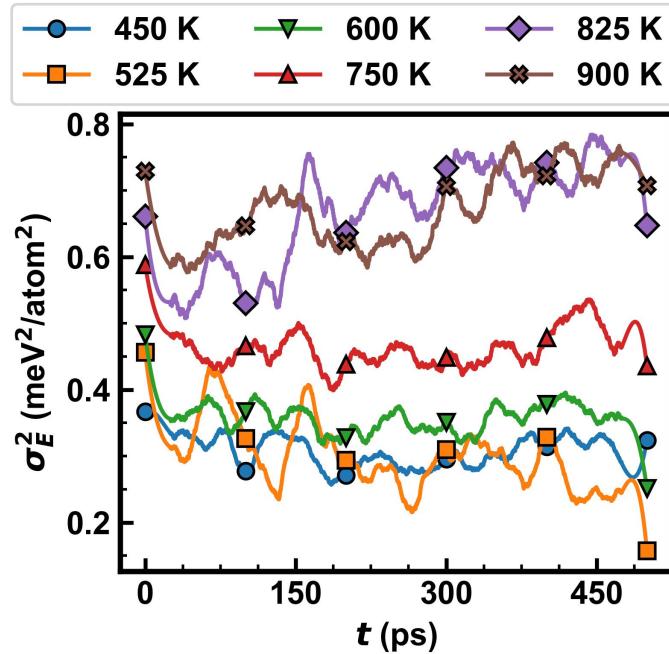


Figure S14: Post processing active learning on a MD trajectory of 83 H₂ molecules over δ-MoC

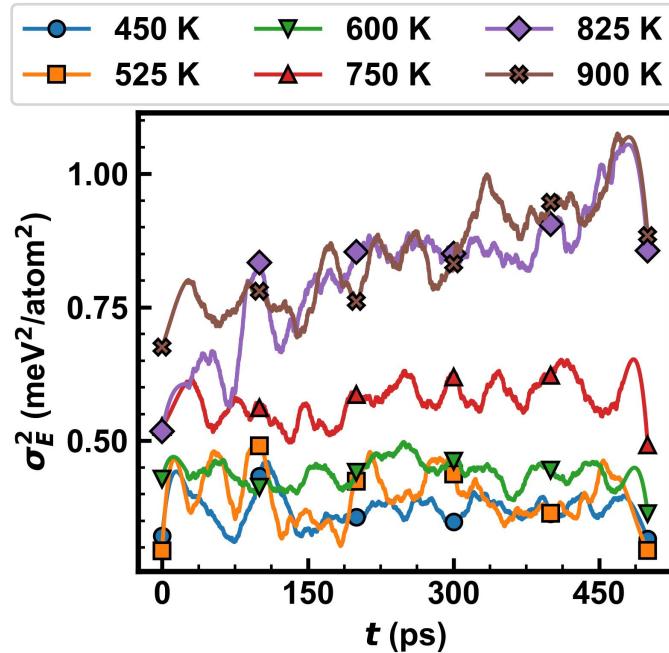


Figure S15: Post processing active learning on a MD trajectory of 124 H₂ molecules over δ-MoC

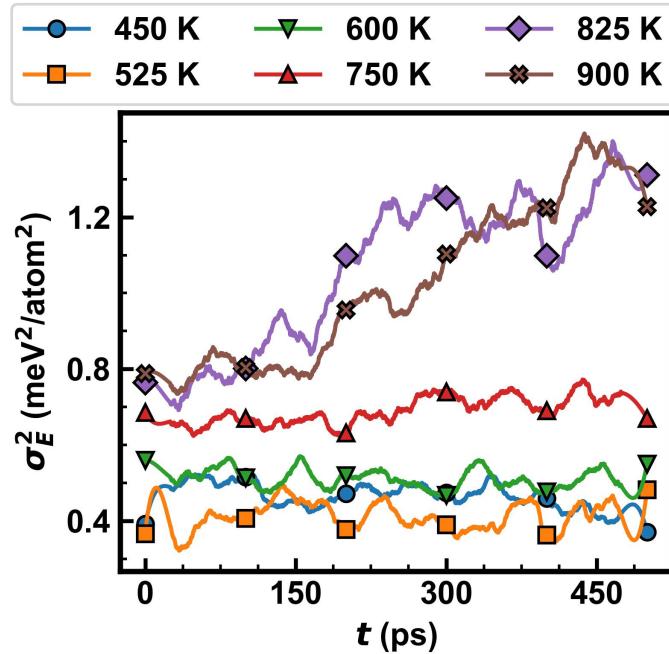


Figure S16: Post processing active learning on a MD trajectory of 25 H₂ molecules over Mo

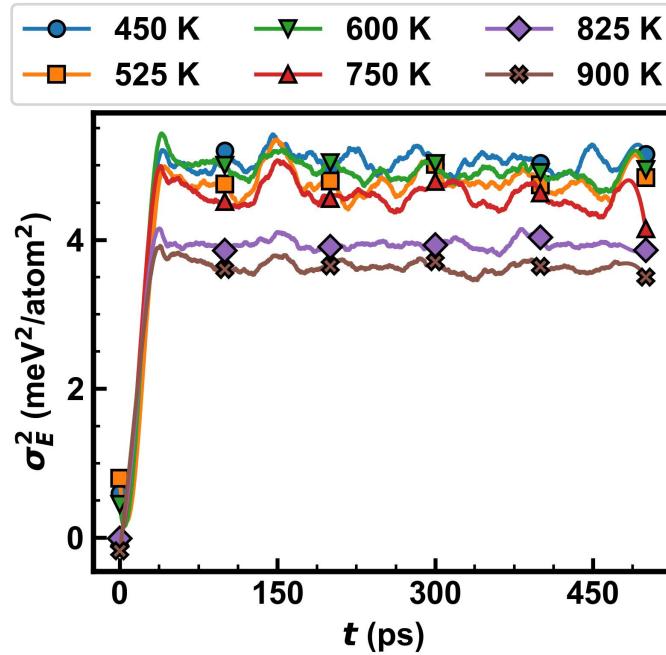


Figure S17: Post processing active learning on a MD trajectory of 29 H₂ molecules over Mo

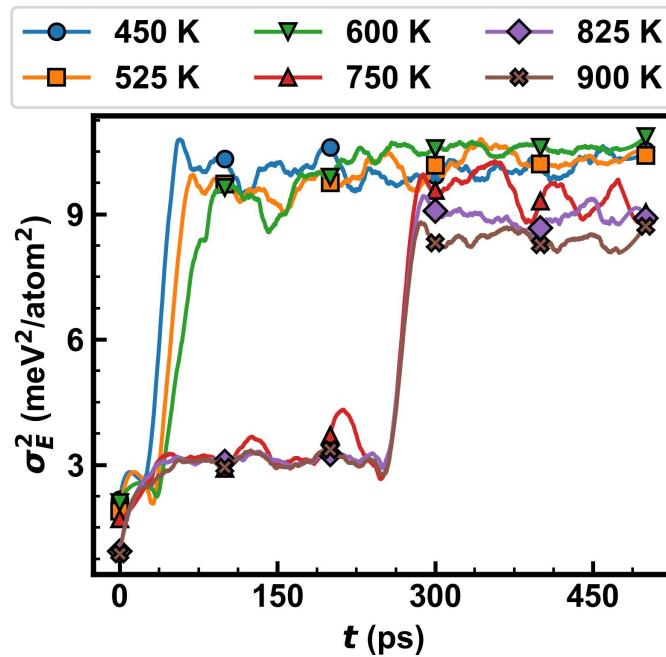


Figure S18: Post processing active learning on a MD trajectory of 61 H₂ molecules over Mo

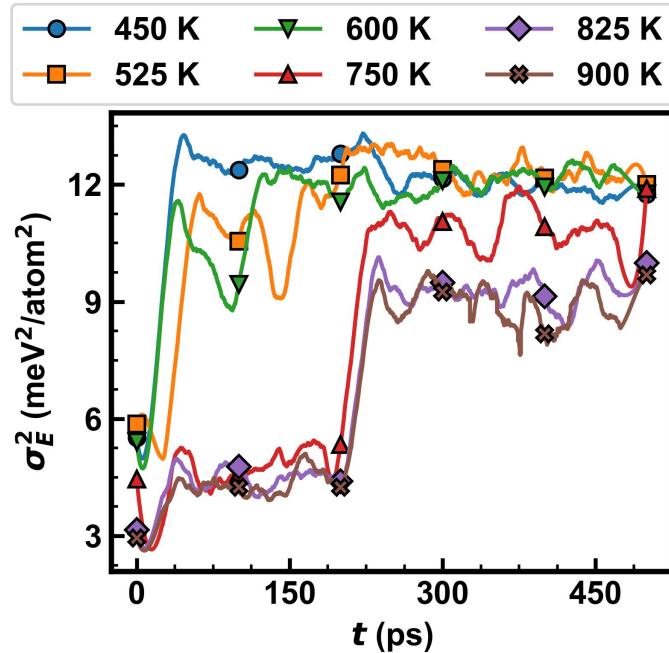


Figure S19: Post processing active learning on a MD trajectory of 85 H₂ molecules over Mo

Table S3: Dissociation reaction rates (ps^{-1}) derived from counting the number of reactions over one periodic surface of material studied

Surface	H_2 Loading	Temperature (K)					
		450	525	600	750	825	900
$\alpha\text{-Mo}_2\text{C } (101)$	90	0.444	0.694	1.692	1.818	2.540	4.547
$\beta\text{-Mo}_2\text{C } (001)$	75	19.633	23.233	29.647	33.028	30.280	35.319
	107	18.707	27.924	32.253	38.200	39.784	42.192
$\delta\text{-MoC Mo-(111)}$	23	0.124	0.438	1.055	1.234	3.579	2.334
	29	0.431	0.782	1.057	2.614	4.840	5.377
	53	1.088	2.815	2.575	5.593	10.432	10.686
	83	4.148	4.797	5.011	11.354	11.354	18.812
	124	4.366	7.420	9.274	14.974	14.974	23.618
Mo (110)	85	NaN	0.007	0.337	0.945	2.800	6.723

Table S4: Recombination reaction rates (ps^{-1}) derived from counting the number of reactions over one periodic surface of material studied

Surface	H_2 Loading	Temperature (K)					
		450	525	600	750	825	900
$\alpha\text{-Mo}_2\text{C } (101)$	90	0.450	0.677	1.692	1.820	2.537	4.541
$\beta\text{-Mo}_2\text{C } (001)$	75	19.624	23.220	29.645	33.028	30.281	35.319
	107	18.705	27.924	32.251	38.205	39.782	42.191
$\delta\text{-MoC Mo-(111)}$	23	0.123	0.437	1.050	1.235	3.580	2.337
	29	0.431	0.783	1.055	2.612	4.840	5.376
	53	1.083	2.811	2.578	5.593	10.430	10.686
	83	4.147	4.803	5.006	11.354	11.354	18.815
	124	4.371	7.418	9.276	14.973	22.183	23.617
Mo (110)	85	NaN	0.007	0.337	0.945	2.807	6.764

Table S5: Recombination activation energy barrier (eV) and log of Arrhenius pre-exponential factor over each catalyst studied

Surface	H ₂ Loading	E _a	ln A
$\alpha\text{-Mo}_2\text{C}$ (101)	90	0.174 ± 0.038	-3.391 ± 0.707
$\beta\text{-Mo}_2\text{C}$ (001)	75	0.058 ± 0.010	-2.587 ± 0.184
	107	0.079 ± 0.010	-2.147 ± 0.189
$\delta\text{-MoC}$ Mo-(111)	23	0.231 ± 0.048	1.774 ± 0.905
	29	0.204 ± 0.024	0.872 ± 0.445
	53	0.174 ± 0.030	1.093 ± 0.558
	83	0.129 ± 0.028	1.020 ± 0.520
	124	0.133 ± 0.011	0.403 ± 0.206
	Mo (110)	85	0.676 ± 0.178
			5.970 ± 3.046

Table S6: Dissociation activation energy barrier (eV) and log of Arrhenius pre-exponential factor over each catalyst studied

Surface	H ₂ Loading	E _a	ln A
$\alpha\text{-Mo}_2\text{C}$ (101)	90	0.148 \pm 0.020	0.871 \pm 0.378
$\beta\text{-Mo}_2\text{C}$ (001)	75	0.070 \pm 0.009	1.076 \pm 0.171
	107	0.056 \pm 0.005	-1.125 \pm 0.088
$\delta\text{-MoC}$ Mo-(111)	23	0.079 \pm 0.022	-0.100 \pm 0.409
	29	0.122 \pm 0.024	0.530 \pm 0.452
	53	0.119 \pm 0.010	0.357 \pm 0.186
	83	0.106 \pm 0.015	0.219 \pm 0.289
	124	0.111 \pm 0.009	0.259 \pm 0.176
	85	0.840 \pm 0.030	-1.125 \pm 0.519

Table S7: Activation energy barrier of diffusion (eV) and log of Arrhenius pre-exponential factor ($\ln \text{Å}/\text{ps}^2$) over each catalyst studied

Surface	E_a	$\ln D_0$
$\alpha\text{-Mo}_2\text{C } (101)$	0.210 ± 0.048	-0.814 ± 0.906
$\beta\text{-Mo}_2\text{C } (001)$	0.290 ± 0.048	-0.017 ± 1.710
$\delta\text{-MoC Mo-(111)}$	0.170 ± 0.035	-0.640 ± 0.661
$\text{Mo } (110)$	0.070 ± 0.026	-2.117 ± 0.488

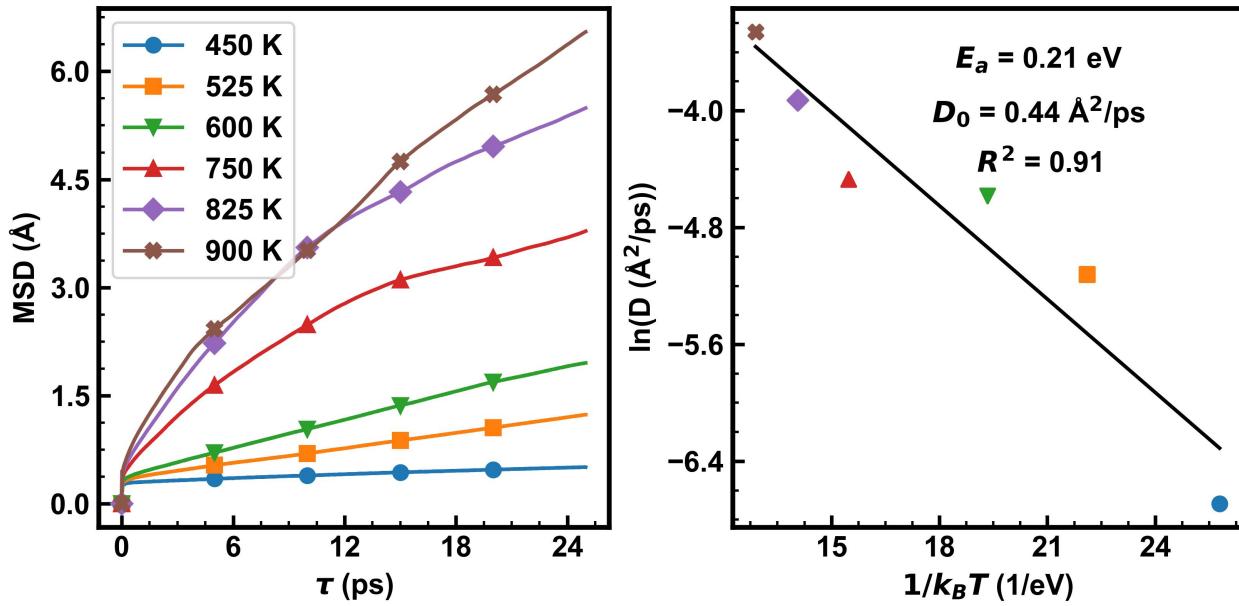


Figure S20: Mean squared displacement and Arrhenius analysis of diffusion of hydrogen on α -Mo₂C (101) at the limit of low coverage.

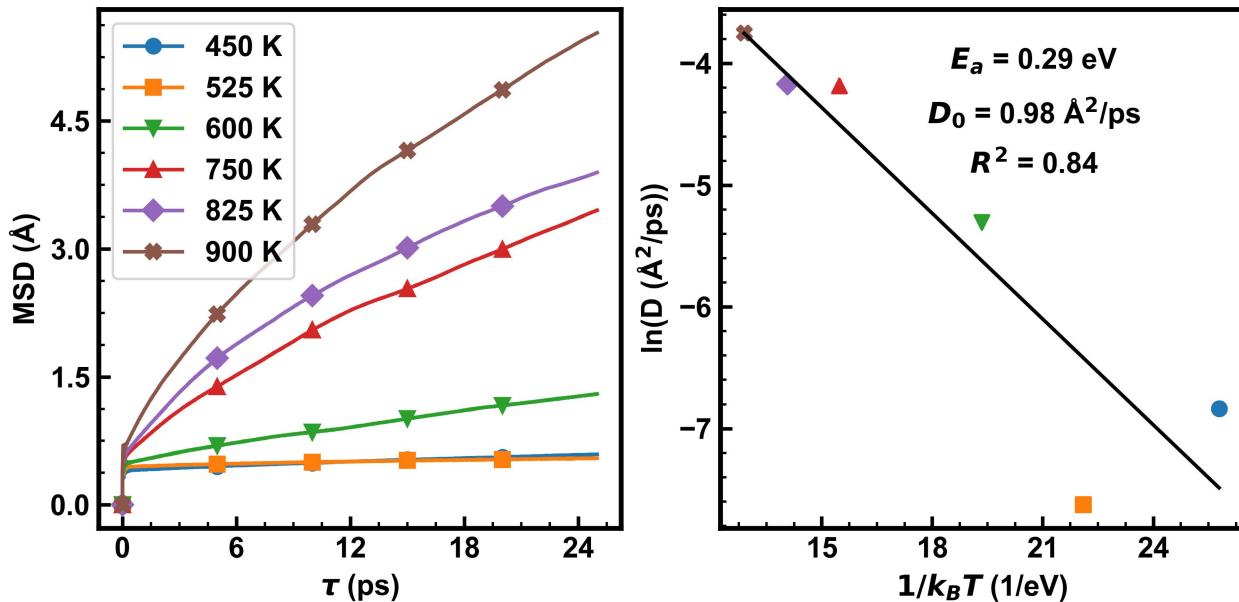


Figure S21: Mean squared displacement and Arrhenius analysis of diffusion of hydrogen on β -Mo₂C (001) at the limit of low coverage.

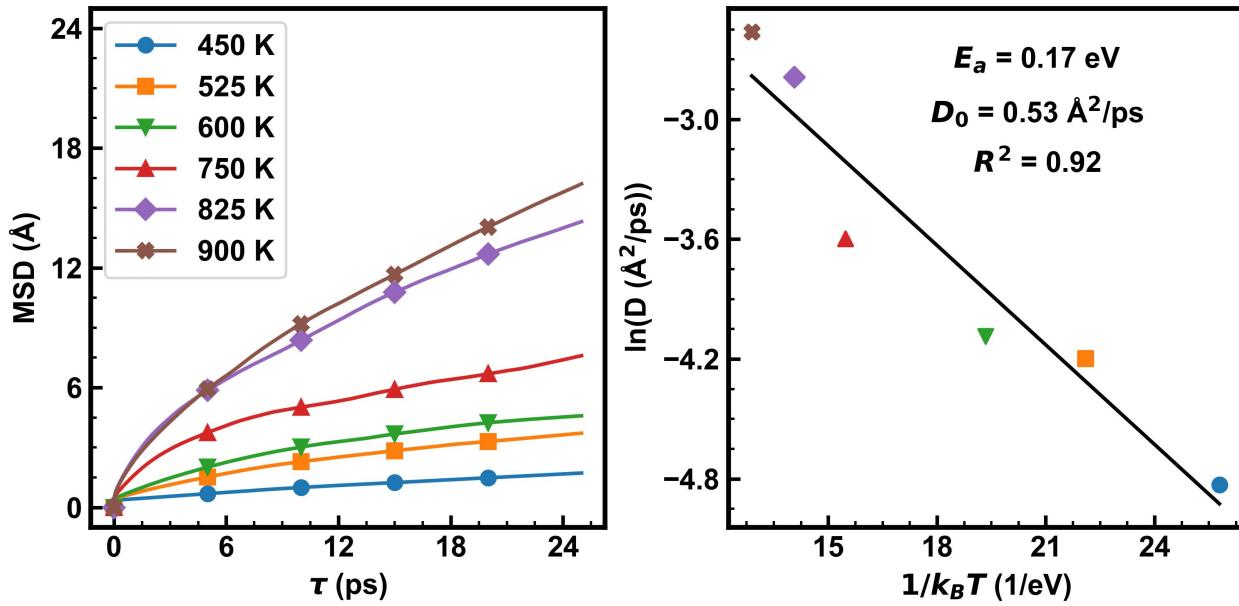


Figure S22: Mean squared displacement and Arrhenius analysis of diffusion of hydrogen on δ -MoC Mo-(111) at the limit of low coverage.

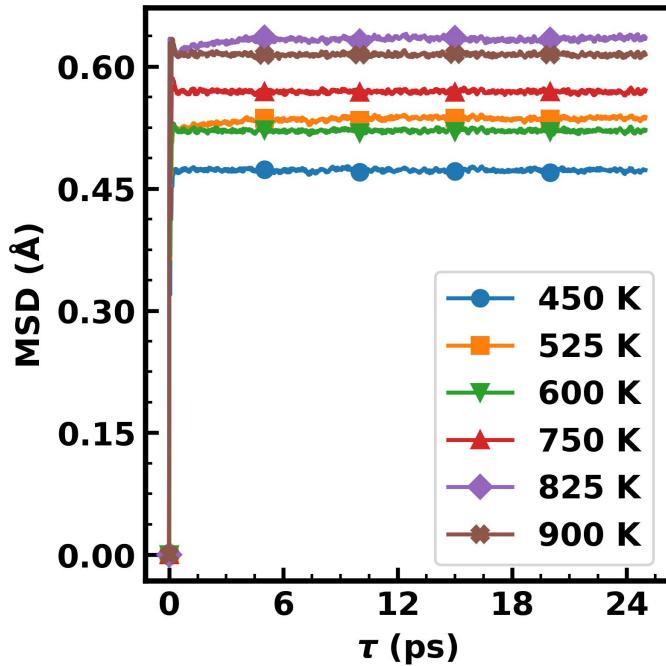


Figure S23: Mean squared displacement and Arrhenius analysis of diffusion of hydrogen on δ -MoC C-(111) at the limit of low coverage.

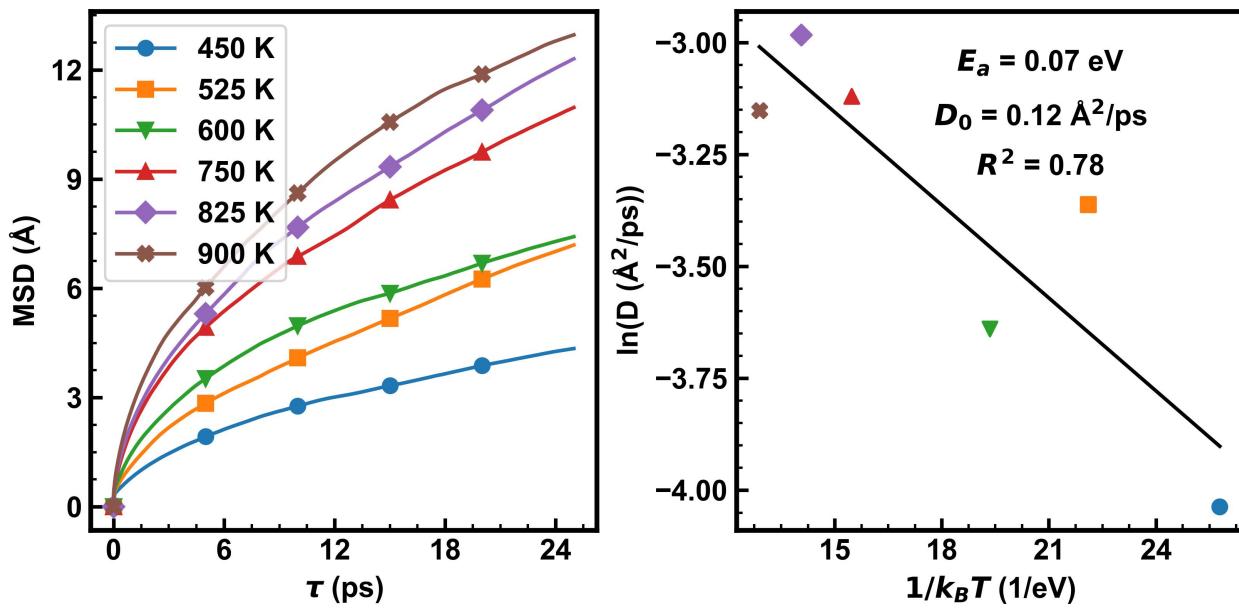


Figure S24: Mean squared displacement and Arrhenius analysis of diffusion of hydrogen on Mo (110) at the limit of low coverage.

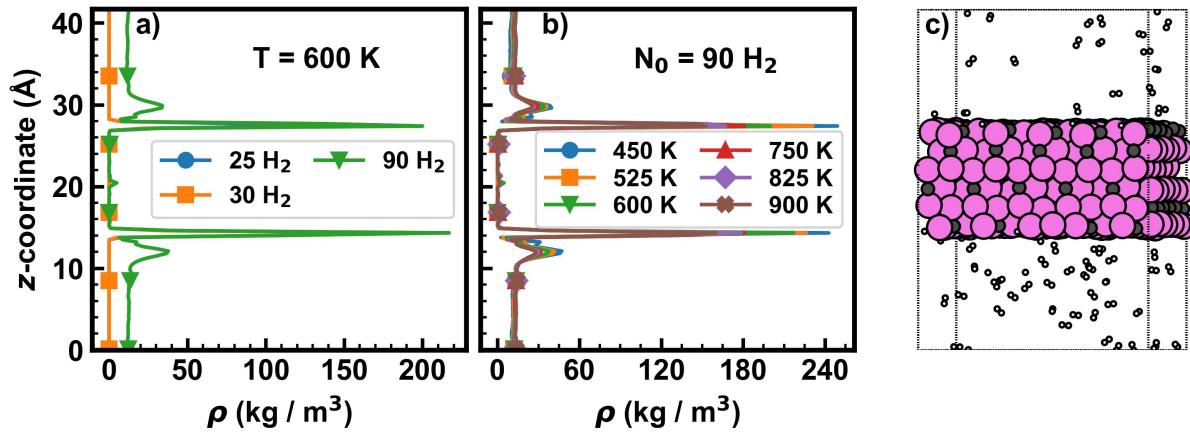


Figure S25: Density profile of hydrogen over $\alpha\text{-Mo}_2\text{C}$ as a function of H_2 loading at 600 K (a), as a function of temperature with 90 H_2 molecules (b), and a simulation snapshot of the last frame of 90 H_2 over $\alpha\text{-Mo}_2\text{C}$ at 900 K (c).

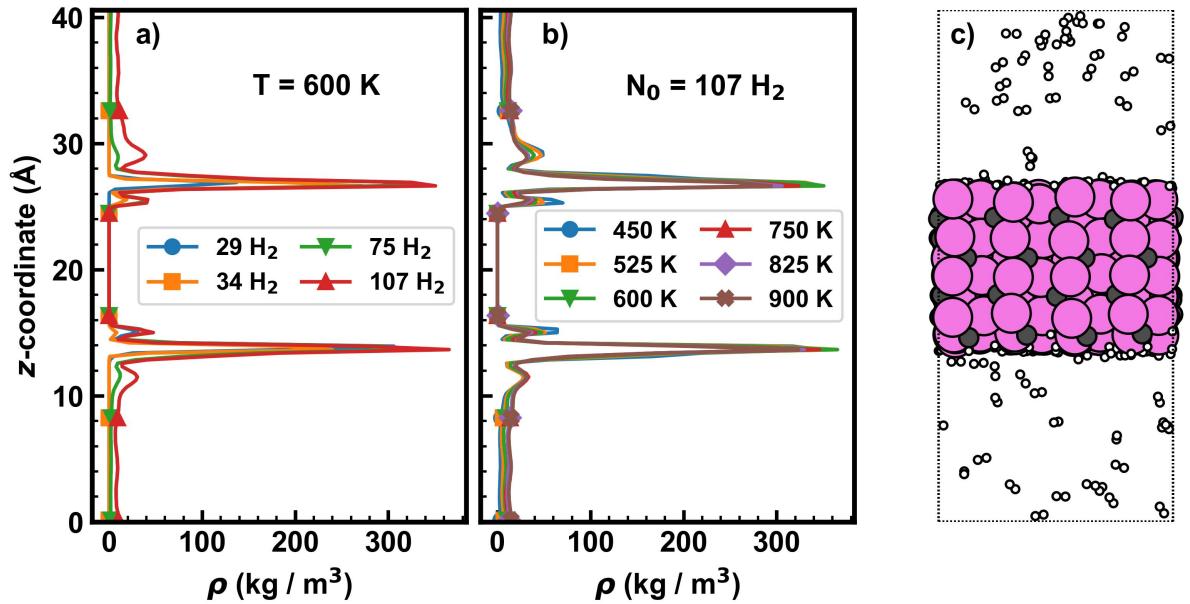


Figure S26: Density profile of hydrogen over $\beta\text{-Mo}_2\text{C}$ as a function of H_2 loading at 600 K (a), as a function of temperature with 107 H_2 molecules (b), and a simulation snapshot of the last frame of 107 H_2 over $\beta\text{-Mo}_2\text{C}$ at 900 K (c).

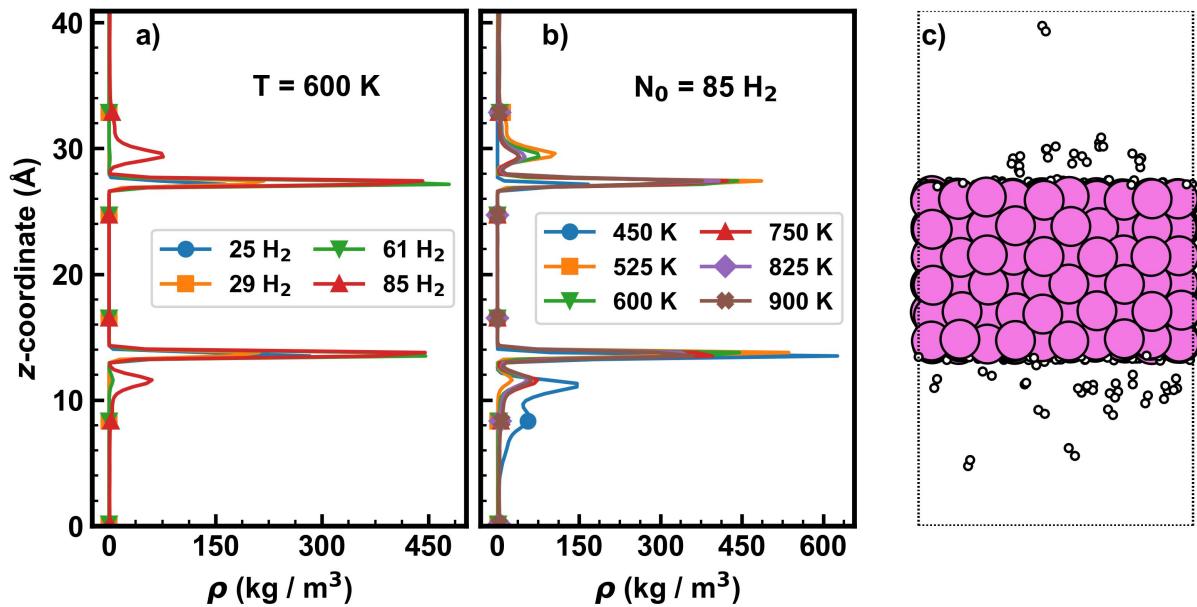


Figure S27: Density profile of hydrogen over Mo as a function of H_2 loading at 600 K (a), as a function of temperature with 124 H_2 molecules (b), and a simulation snapshot of the last frame of 124 H_2 over Mo at 900 K (c).

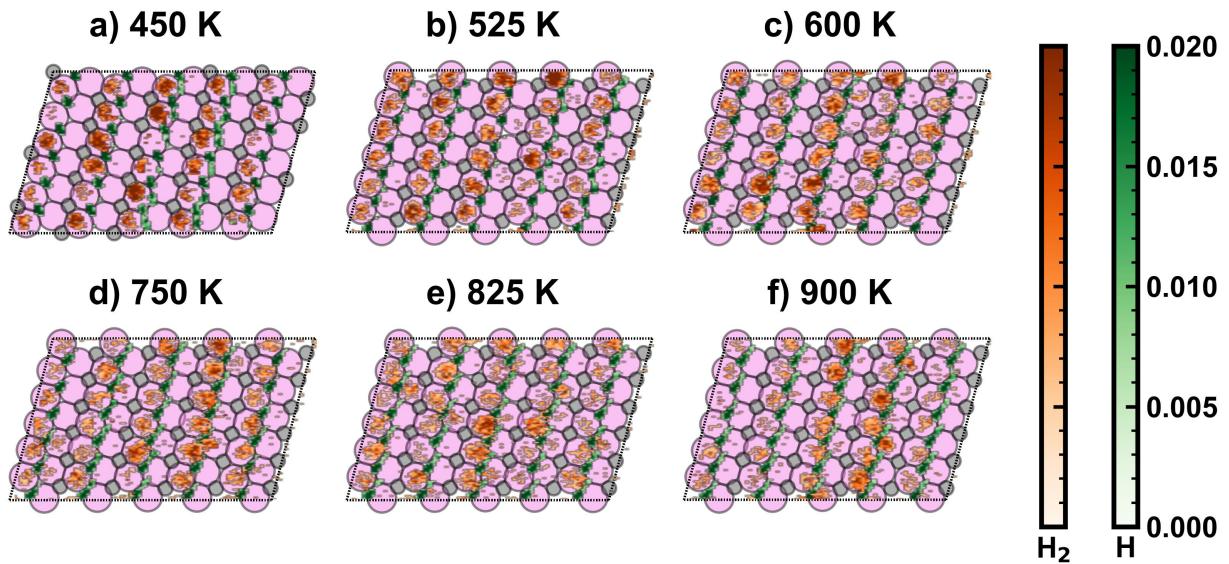


Figure S28: Molecular and atomic hydrogen adsorption probability heat maps for the α - Mo_2C (101) surface with 90 H_2 molecules

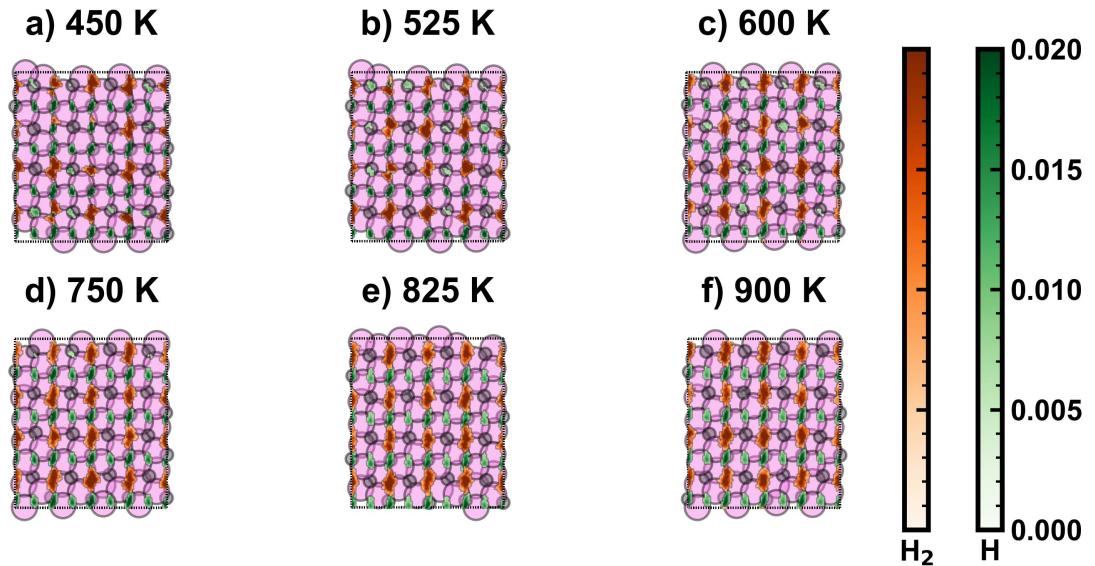


Figure S29: Molecular and atomic hydrogen adsorption probability heat maps for the β - Mo_2C (001) surface with 107 H_2 molecules

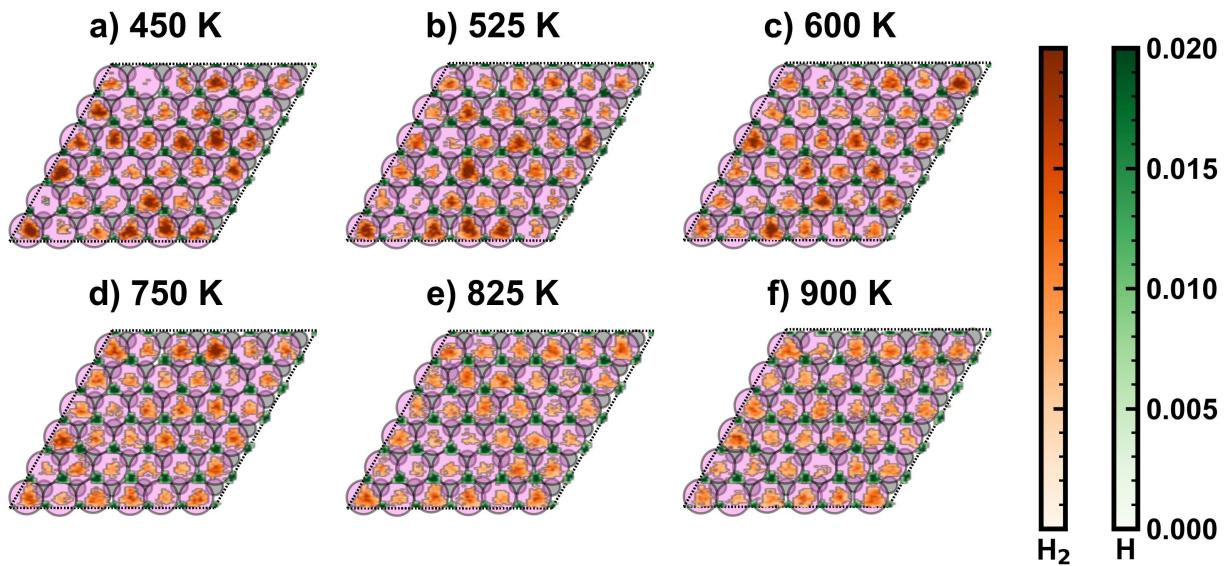


Figure S30: Molecular and atomic hydrogen adsorption probability heat maps for the δ -MoC Mo-(111) surface with 124 H_2 molecules

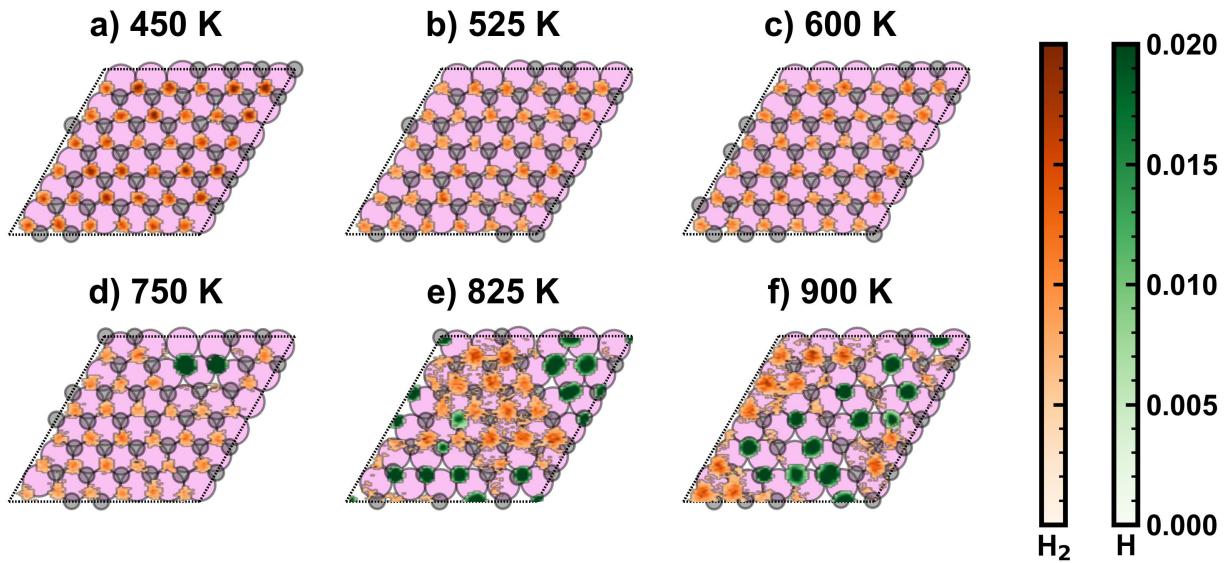


Figure S31: Molecular and atomic hydrogen adsorption probability heat maps for the δ -MoC C-(111) surface with 124 H_2 molecules

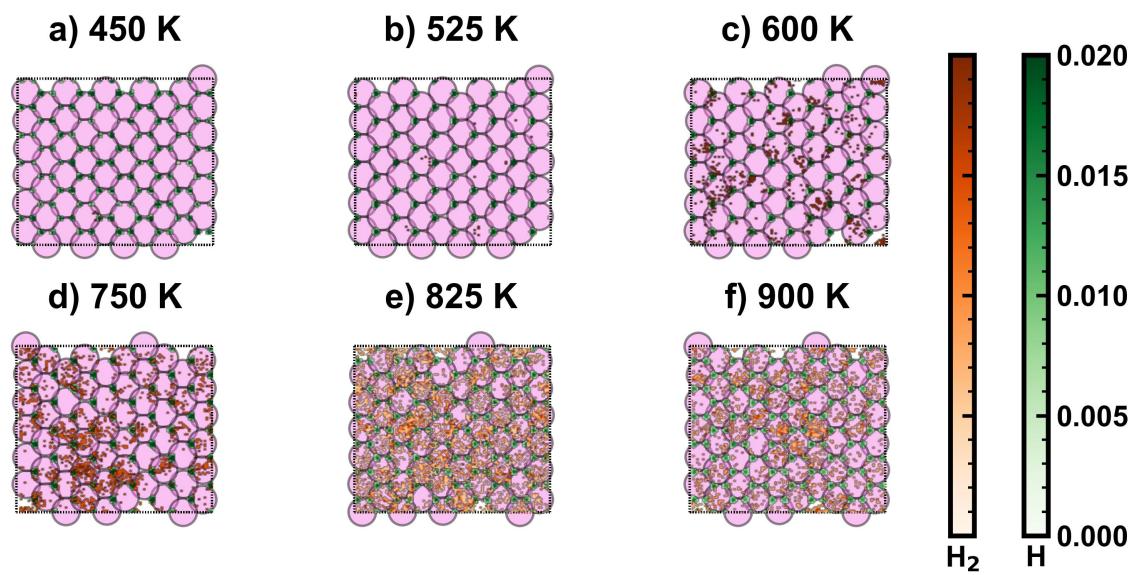


Figure S32: Molecular and atomic hydrogen adsorption probability heat maps for the $\text{Mo}(110)$ surface with 85 H_2 molecules