Supporting information for

Comparative Theoretical Study on the Vibrational Spectra of $V_2O_5 \cdot nH_2O$

Shuang Yu[1], Xiaodong Zhang[1], Qiang Zhan[1], Hao Yu[1], Bo Zhou[1*]

* E-mail:zhoubo@nwu.edu.cn

[1]Institute of Modern Physics, Shanxi Key Laboratory for Theoretical Physics Frontiers, Northwest University, Xi'an 710127, People's Republic of China.

Table S1: Optimized structures of $V_2O_5 \cdot H_2O$ unit cell after two types of optimizations: (1) a symmetry-constrained optimization within the C2/m space group, and (2) a symmetry-unconstrained optimization in P1. All the positions are in fractional coordinates.

Model		C2/m			P1	
a, b, c (Å)	11.69	3.63	10.80	11.69	3.63	10.93
α, β, γ (deg.)	90.0	91.3	90.0	90.0	88.5	90.0
	x/a	y/b	z/c	x/a	y/b	z/c
V(1)	0.9385	0.0000	0.1441	0.9316	1.0000	0.1411
V(2)	0.0615	0.0000	0.8559	0.0684	0.0000	0.8589
V(3)	0.4385	0.5000	0.1441	0.4316	0.5000	0.1411
V(4)	0.5615	0.5000	0.8559	0.5684	0.5000	0.8589
V(5)	0.2279	0.0000	0.1456	0.2213	0.0000	0.1437
V(6)	0.7721	0.0000	0.8544	0.7787	1.0000	0.8563
V(7)	0.7279	0.5000	0.1456	0.7212	0.5000	0.1437
V(8)	0.2721	0.5000	0.8544	0.2787	0.5000	0.8563
O(1)	0.3976	0.0000	0.1176	0.3918	0.0000	0.1152
O(2)	0.6024	0.0000	0.8824	0.6082	1.0000	0.8848
O(3)	0.8976	0.5000	0.1176	0.8918	0.5000	0.1152
O(4)	0.1024	0.5000	0.8824	0.1082	0.5000	0.8848
O(5)	0.0823	0.0000	0.0829	0.0788	0.0000	0.0814
O(6)	0.9177	0.0000	0.9171	0.9212	0.0000	0.9186
O(7)	0.5823	0.5000	0.0829	0.5788	0.5000	0.0814
O(8)	0.4177	0.5000	0.9171	0.4212	0.5000	0.9186
O(9)	0.7623	0.0000	0.1091	0.7569	1.0000	0.1077
O(10)	0.2377	0.0000	0.8909	0.2431	0.0000	0.8923
O(11)	0.2623	0.5000	0.1091	0.2569	0.5000	0.1077
O(12)	0.7377	0.5000	0.8909	0.7431	0.5000	0.8923
O(13)	0.2119	0.0000	0.2907	0.1985	0.0001	0.2873
O(14)	0.7881	0.0000	0.7093	0.8014	0.9999	0.7127
O(15)	0.7119	0.5000	0.2907	0.6986	0.4999	0.2873
O(16)	0.2881	0.5000	0.7093	0.3015	0.5002	0.7127
O(17)	0.9611	0.0000	0.2896	0.9478	0.9999	0.2845
O(18)	0.0389	0.0000	0.7104	0.0522	0.0001	0.7155
O(19)	0.4611	0.5000	0.2896	0.4478	0.5001	0.2845

O(20)	0.5389	0.5000	0.7104	0.5522	0.5000	0.7155
O(21)	0.6406	0.0000	0.5028	0.6493	0.9985	0.5117
O(22)	0.3594	0.0000	0.4972	0.3507	0.0020	0.4883
O(23)	0.1406	0.5000	0.5028	0.1493	0.5020	0.5117
O(24)	0.8594	0.5000	0.4972	0.8507	0.4985	0.4883
H(1)	0.5820	0.0000	0.4367	0.5977	0.9997	0.4430
H(2)	0.4180	0.0000	0.5633	0.4023	0.0003	0.5570
H(3)	0.0820	0.5000	0.4367	0.0977	0.5004	0.4430
H(4)	0.9180	0.5000	0.5633	0.9023	0.4998	0.5570
H(5)	0.7142	0.0000	0.4609	0.7267	0.0020	0.4745
H(6)	0.2858	0.0000	0.5391	0.2733	0.9972	0.5255
H(7)	0.2142	0.5000	0.4609	0.2267	0.4972	0.4745
H(8)	0.7858	0.5000	0.5391	0.7733	0.5020	0.5255

Table S2: Lattice parameters and atomic positions of the optimized $V_2O_5 \cdot 2H_2O$ structure used in vibrational property calculations. All the positions are in fractional coordinates.

Model		P1	
a, b, c (Å)	11.74	3.61	13.07
α, β, γ (deg.)	90.1	90.1	90.0
	x/a	y/b	z/c
V(1)	0.9350	0.0014	0.1188
V(2)	0.0649	0.9998	0.8813
V(3)	0.4350	0.5004	0.1186
V(4)	0.5650	0.4990	0.8812
V(5)	0.2254	0.9995	0.1195
V(6)	0.7746	0.9981	0.8799
V(7)	0.7254	0.5021	0.1201
V(8)	0.2746	0.5007	0.8805
O(1)	0.3952	0.0000	0.0943
O(2)	0.6048	0.9988	0.9055
O(3)	0.8952	0.5015	0.0945
O(4)	0.1047	0.5002	0.9056
O(5)	0.0801	0.0012	0.0712
O(6)	0.9197	0.0003	0.9285

O(7)	0.5803	0.5000	0.0715
O(8)	0.4199	0.4991	0.9288
O(9)	0.7604	0.0015	0.0879
O(10)	0.2397	0.0004	0.9126
O(11)	0.2603	0.4998	0.0874
O(12)	0.7396	0.4988	0.9121
O(13)	0.2131	0.9994	0.2401
O(14)	0.7868	0.9968	0.7593
O(15)	0.7132	0.5034	0.2407
O(16)	0.2869	0.5008	0.7599
O(17)	0.9479	0.0021	0.2397
O(18)	0.0526	0.9992	0.7603
O(19)	0.4473	0.5010	0.2396
O(20)	0.5522	0.4982	0.7603
O(21)	0.5858	0.0177	0.3831
O(22)	0.6359	0.9762	0.5797
O(23)	0.3623	0.9795	0.4198
O(24)	0.4123	0.0134	0.6167
O(25)	0.0880	0.4862	0.3834
O(26)	0.1376	0.5183	0.5804
O(27)	0.8644	0.5251	0.4201
O(28)	0.9139	0.4824	0.6168
H(1)	0.4996	0.0095	0.3881
H(2)	0.6261	0.9792	0.5025
H(3)	0.3721	0.9800	0.4971
H(4)	0.4986	0.0055	0.6117
H(5)	0.0017	0.4948	0.3883
H(6)	0.1280	0.5182	0.5031
H(7)	0.8740	0.5216	0.4974
H(8)	0.0002	0.4897	0.6120
H(9)	0.6060	0.2678	0.3601
H(10)	0.6681	0.7340	0.5975
H(11)	0.3297	0.7385	0.4013
H(12)	0.3921	0.2632	0.6401
H(13)	0.1081	0.2364	0.3599
H(14)	0.1702	0.7592	0.5990
H(15)	0.8323	0.7674	0.4023
H(16)	0.8934	0.2325	0.6397

Table S3: Lattice parameters and atomic positions of the optimized $V_2O_5 \cdot 0.5H_2O$ structure used in vibrational property calculations. All the positions are in fractional coordinates.

Model		P1	
a, b, c (Å)	11.84	3.63	9.37
α, β, γ (deg.)	89.2	94.4	90.2

	x/a	y/b	z/c
V(1)	0.9386	-0.0017	0.1574
V(2)	0.2357	-0.0048	0.1663
V(3)	0.4436	0.4981	0.1640
V(4)	0.7332	0.4983	0.1553
V(5)	0.0565	0.0056	0.8376
V(6)	0.7591	0.0115	0.8249
V(7)	0.5528	0.5070	0.8350
V(8)	0.2637	0.5080	0.8451
O(1)	0.4024	-0.0016	0.1313
O(2)	0.0842	-0.0009	0.1086
O(3)	0.7642	-0.0003	0.1096
O(4)	0.2454	-0.0118	0.3361
O(5)	0.9429	-0.0067	0.3271
O(6)	0.9001	0.5000	0.1191
O(7)	0.5838	0.4991	0.0964
O(8)	0.2672	0.4975	0.1211
O(9)	0.7329	0.4944	0.3248
O(10)	0.4677	0.4922	0.3331
O(11)	0.0963	0.4829	0.4408
O(12)	0.5928	0.0068	0.8684
O(13)	0.9110	0.0064	0.8839
O(14)	0.2331	0.0059	0.8908
O(15)	0.7422	0.0167	0.6561
O(16)	0.0591	0.0077	0.6687
O(17)	0.0972	0.5050	0.8774
O(18)	0.4125	0.5055	0.9051
O(19)	0.7277	0.5083	0.8735
O(20)	0.2653	0.5172	0.6750
O(21)	0.5260	0.5123	0.6664

O(22)	0.8986	0.5115	0.5873
H(1)	0.0955	0.2135	0.4458
H(2)	0.1603	0.5510	0.5082
H(3)	0.9666	0.5153	0.5313
H(4)	0.8416	0.6501	0.5285

Table S4: Lattice parameters and atomic positions of the optimized $V_2O_5 \cdot 2H_2O$ structure used in vibrational property calculations. All the positions are in fractional coordinates.

Model		P1	
a, b, c (Å)	11.73	3.65	12.35
α, β, γ (deg.)	88.8	86.5	90.1

	x/a	y/b	z/c
V(1)	0.9273	0.9893	0.1114
V(2)	0.0726	0.0130	0.8615
V(3)	0.4246	0.4917	0.1093
V(4)	0.5752	0.5098	0.8645
V(5)	0.2179	0.9886	0.1104
V(6)	0.7819	0.0128	0.8642
V(7)	0.7192	0.4880	0.1140
V(8)	0.2808	0.5142	0.8585
O(1)	0.3883	0.9929	0.0833
O(2)	0.6116	0.0087	0.8907
O(3)	0.8901	0.4906	0.0872
O(4)	0.1101	0.5116	0.8857
O(5)	0.0759	0.9952	0.0592
O(6)	0.9244	0.0069	0.9143
O(7)	0.5754	0.4931	0.0650
O(8)	0.4242	0.5087	0.9082
O(9)	0.7553	0.9905	0.0806
O(10)	0.2447	0.0117	0.8917
O(11)	0.2531	0.4923	0.0765
O(12)	0.7467	0.5094	0.8979
O(13)	0.1950	0.9758	0.2380

O(14)	0.8046	0.0252	0.7361
O(15)	0.7037	0.4752	0.2420
O(16)	0.2966	0.5266	0.7304
O(17)	0.9362	0.9794	0.2391
O(18)	0.0632	0.0228	0.7341
O(19)	0.4207	0.4826	0.2375
O(20)	0.5798	0.5185	0.7361
O(21)	0.5521	0.9723	0.3536
O(22)	0.6616	0.0233	0.5347
O(23)	0.3395	0.9728	0.4384
O(24)	0.4492	0.0264	0.6193
O(25)	0.1738	0.4625	0.4473
O(26)	0.8263	0.5337	0.5303
H(1)	0.4670	0.9743	0.3762
H(2)	0.6285	-0.0157	0.4620
H(3)	0.3728	0.0141	0.5108
H(4)	0.5341	0.0238	0.5968
H(5)	0.1206	0.5128	0.3911
H(6)	0.8744	0.4842	0.5907
H(7)	0.5692	0.2240	0.3285
H(8)	0.7198	0.8221	0.5445
H(9)	0.2808	0.1729	0.4291
H(10)	0.4313	0.7743	0.6443
H(11)	0.2289	0.6748	0.4454
H(12)	0.7708	0.3224	0.5292

Table S5： Comparison of lattice parameters for $V_2O_5 \cdot nH_2O$ models optimized using the **MACE** neural network potential and DFT calculation in this work. Experimental data for $V_2O_5 \cdot H_2O$ are denoted as "Exp.[1]"

	model	a	b	c	α	β	γ
MACE large MODEL	$V_2O_5 \cdot 0.5H_2O$	11.81	3.68	13.27	91.73	93.83	90.05
	$V_2O_5 \cdot H_2O$	11.77	3.72	13.33	90.01	87.66	90.00
	$V_2O_5 \cdot 1.5H_2O$	11.74	3.71	15.48	85.17	92.74	90.20
	$V_2O_5 \cdot 2H_2O$	11.74	3.72	15.26	92.01	93.6	90.09
DFT in	$V_2O_5 \cdot 0.5H_2O$	11.84	3.63	9.37	89.21	94.36	90.17

this	$V_2O_5·H_2O$	11.69	3.64	10.93	90.00	88.48	90.00
work	$V_2O_5·1.5H_2O$	11.73	3.65	12.35	88.80	86.53	90.05
	$V_2O_5·2H_2O$	11.74	3.61	13.07	90.08	90.12	90.00
Exp.[1]	V2O5·H_2O	11.72	3.57	11.52	90.00	88.65	90.00

Table S6: Vibrational modes of hydrated V_2O_5 with different water contents calculated using the **MACE** neural network potential. Characteristic Raman peaks are highlighted in yellow.

mode	$V_2O_5·0.5H_2O$	$V_2O_5·H_2O$	$V_2O_5·1.5H_2O$	$V_2O_5·2H_2O$
1	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0
4	38.3	15.7	22.7	28.6
5	46.4	36.8	37.3	29.8
6	48.0	44.6	38.9	39.0
7	52.0	46.5	47.7	43.7
8	52.9	51.7	50.7	48.3
9	55.4	53.7	51.4	49.3
10	59.0	55.1	54.0	50.0
11	60.3	59.1	55.5	54.2
12	63.3	63.4	56.1	61.4
13	67.2	66.0	62.3	63.8
14	70.3	67.5	62.8	64.5
15	76.4	68.2	67.3	66.8
16	78.7	69.1	69.5	67.5
17	87.4	70.4	71.7	69.7
18	90.2	72.0	73.3	70.2
19	95.8	76.8	77.6	71.8
20	100.4	80.9	78.7	72.3
21	111.1	101.9	82.6	78.0
22	117.8	108.4	88.7	81.0
23	127.7	112.2	90.7	85.0
24	128.5	120.6	94.8	88.3
25	132.4	120.8	104.1	98.1
26	133.7	129.4	108.9	98.7
27	136.9	131.4	116.1	103.0

28	138.8	133.4	118.0	112.1
29	147.0	133.8	122.1	117.5
30	150.3	134.5	130.9	120.7
31	171.0	135.9	132.6	120.8
32	172.5	139.4	134.7	125.2
33	176.0	150.1	137.9	130.6
34	177.1	152.9	140.1	132.4
35	179.4	159.0	141.3	135.7
36	183.0	159.3	162.1	137.0
37	184.8	166.9	165.1	141.1
38	187.0	178.6	167.1	148.6
39	191.8	178.7	173.8	158.9
40	193.6	182.6	175.6	162.0
41	194.3	184.8	179.0	167.3
42	194.9	185.5	183.6	172.0
43	195.6	187.4	183.8	174.1
44	196.6	189.6	185.4	179.3
45	197.7	190.1	187.1	182.0
46	202.3	192.8	190.5	184.4
47	202.8	192.9	192.2	188.3
48	207.2	199.1	192.8	191.7
49	213.6	201.1	194.3	192.0
50	215.9	201.7	195.2	193.8
51	217.1	206.4	196.0	194.7
52	220.4	208.5	200.5	195.1
53	224.4	212.3	200.9	197.3
54	225.6	215.0	205.6	200.0
55	226.4	218.9	212.7	201.0
56	239.0	220.5	214.3	209.0
57	241.3	227.0	214.5	211.0
58	241.4	227.9	216.1	211.9
59	245.2	228.8	221.1	213.3
60	251.9	233.3	222.3	215.1
61	254.6	234.7	229.5	216.4
62	260.2	240.5	237.6	218.2
63	263.4	245.4	240.7	220.8
64	267.8	248.4	243.7	223.7
65	277.9	252.1	244.9	230.2

66	278.9	260.5	247.0	237.9
67	282.5	260.7	250.8	240.5
68	288.2	265.0	251.9	241.0
69	290.5	269.3	255.8	243.0
70	293.9	272.0	259.1	244.3
71	300.5	273.2	260.7	247.1
72	304.5	278.7	266.7	253.0
73	308.6	286.3	268.7	259.8
74	327.0	288.9	277.2	260.2
75	328.0	294.3	279.3	261.5
76	353.2	297.3	282.8	265.8
77	368.7	300.3	284.7	269.5
78	370.6	304.7	288.5	275.1
79	380.0	313.9	296.0	284.4
80	387.3	333.3	299.4	285.0
81	390.5	354.2	304.9	289.9
82	394.0	361.9	306.2	292.7
83	401.0	375.4	311.1	297.6
84	403.3	376.5	311.2	298.9
85	407.9	378.2	319.5	301.7
86	468.2	387.1	338.4	306.3
87	525.2	388.9	339.8	316.8
88	624.8	394.9	342.7	322.8
89	957.4	427.3	361.9	326.7
90	977.3	430.0	364.0	342.4
91	986.6	442.0	377.9	344.0
92	995.3	443.3	380.2	347.6
93	997.6	503.9	383.6	362.0
94	1015.7	509.3	395.6	367.7
95	1030.4	635.7	395.7	378.2
96	1034.1	636.0	398.8	389.3
97	1466.7	643.4	400.4	390.8
98	1506.4	643.9	405.5	392.4
99	3406.1	962.6	464.1	395.4
100	3484.0	967.5	466.9	396.4
101	3705.7	970.3	500.7	429.7
102	3714.5	974.9	513.2	431.2
103		984.6	649.4	446.8

104	986.8	673.2	451.3
105	990.9	704.2	517.6
106	993.8	730.6	530.9
107	1010.6	741.2	560.6
108	1011.2	767.7	568.6
109	1441.3	875.2	594.3
110	1443.4	961.6	618.8
111	1533.3	965.2	637.1
112	1535.7	969.4	666.1
113	2925.6	980.7	680.4
114	2936.5	986.3	710.2
115	3085.0	999.5	759.7
116	3101.0	1002.4	768.7
117	3603.7	1019.2	809.9
118	3606.9	1022.4	862.5
119	3623.4	1089.5	908.8
120	3626.6	1109.1	940.7
121		1487.3	950.0
122		1491.1	950.7
123		1506.8	960.7
124		1520.1	962.5
125		1575.1	981.1
126		1578.0	1008.0
127		2868.6	1011.0
128		2895.3	1015.4
129		3050.9	1021.3
130		3075.7	1022.4
131		3118.0	1127.5
132		3132.4	1135.3
133		3177.8	1483.4
134		3208.9	1496.3
135		3672.6	1505.4
136		3680.0	1506.5
137		3687.4	1515.7
138		3690.9	1535.9
139			1581.1
140			1591.7
141			2802.9

142	2816.8
143	2906.4
144	2921.0
145	2968.1
146	2999.9
147	3030.3
148	3056.3
149	3235.0
150	3238.2
151	3250.8
152	3254.7
153	3574.5
154	3575.8
155	3596.8
156	3600.5

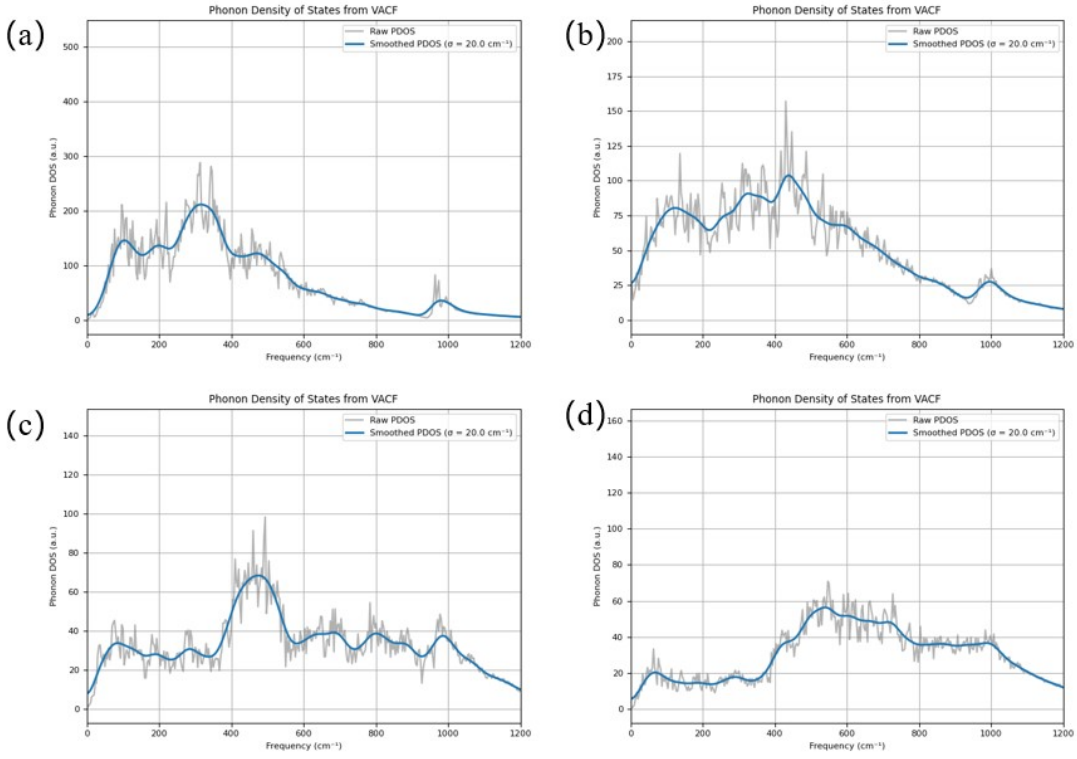

Figure S1: Vibrational densities of states (VDOS) of 3×3×3 supercell models calculated using the MACE neural network potential for (a) $V_2O_5 \cdot 0.5H_2O$, (b) $V_2O_5 \cdot H_2O$, (c) $V_2O_5 \cdot 1.5H_2O$, and (d) $V_2O_5 \cdot 2H_2O$.

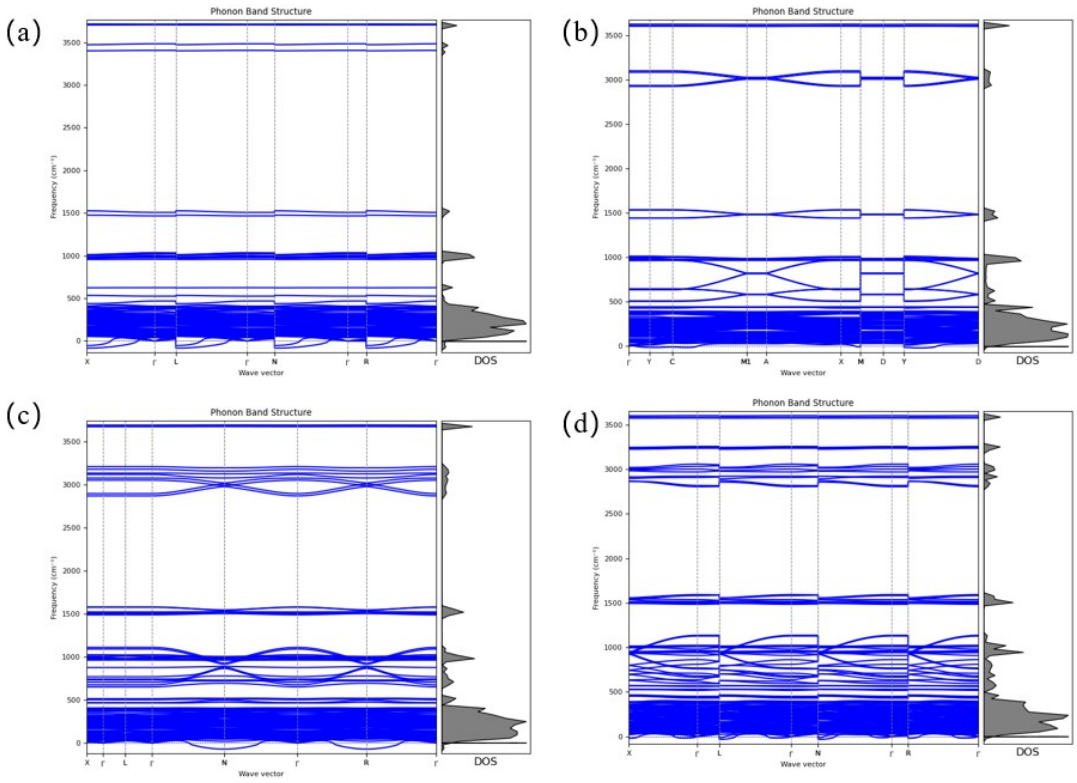

Figure S2: Calculated phonon dispersions of $V_2O_5 \cdot nH_2O$ using the MACE neural network potential at different water contents in (a) 0.5, (b) 1.0, (c) 1.5 and (d) 2.0 along high-symmetry lines.

Source code S1: Python script used for structural optimization and finite-displacement phonon calculations based on the MACE neural network potential.

```
import torch

from ase.io import read
from mace.calculators import mace_mp

from ase.build import bulk
from ase.phonons import Phonons

from ase.optimize import BFGS
from ase.filters import FrechetCellFilter
```

```
import matplotlib.pyplot as plt

import warnings
warnings.filterwarnings("ignore", category=UserWarning)

# Setup crystal and EMT calculator
atoms = read("POSCAR")
print(f" primitive unit cell: {len(atoms)} atoms, chemical formula
{atoms.get_chemical_formula()}")

# Optional: small, medium, large (larger for greater accuracy)
model="large"

print(f" Load the mace-mp model（{model}）...")
calc = mace_mp(
    model,
    device='cpu' if torch.cuda.is_available() else 'cpu',
    default_dtype="float64"     # Essential for high-precision phonons!
)

atoms.calc = calc
# Step 2: First optimize the atomic positions (fixed unit cell, ISIF=2 equivalent)
print("=1=Optimize atomic positions (fixed unit cell)===")
dyn_pos = BFGS(atoms, logfile='opt_pos.log')
dyn_pos.run(fmax=0.005)  # Convergence criterion: 0.005 eV/Å

# Save the optimized structure
atoms.write('POSCAR_pos_opt', format='vasp')

# Cell optimization (volume + shape + position, ISIF=3 equivalent)
print("=2= Optimize the unit cell (volume + shape + position) ===")
ecf = FrechetCellFilter(atoms, scalar_pressure=0.0)  # 0 GPa pressure
dyn_cell = BFGS(ecf, logfile='opt_cell.log')
dyn_cell.run(fmax=0.005)  # Same convergence criteria as above

# Save the fully optimized structure (recommended for subsequent phonon calculations).
atoms_opt = atoms.copy()  # Optimized structure
```

```
atoms_opt.write('POSCAR_opt_1', format='vasp')

print("=3= Further optimize the unit cell (volume + shape + position) ===")
atoms_opt.calc = calc
ecf = FrechetCellFilter(atoms_opt, scalar_pressure=0.0)    # 0 GPa pressure
dyn_cell = BFGS(ecf, logfile='opt_cell.log')
dyn_cell.run(fmax=0.005)    # Same convergence criteria as above

# Save the fully optimized structure (recommended for subsequent phonon calculations)
atoms_opt2 = atoms_opt.copy()    # Optimized structure
atoms_opt2.write('POSCAR_opt_2', format='vasp')



print("Optimization complete! Final cell parameters：")
#print(atoms_opt2.cell)

a = atoms_opt2.cell.lengths()[0]
b = atoms_opt2.cell.lengths()[1]
c = atoms_opt2.cell.lengths()[2]
alpha, beta, gamma = atoms_opt2.cell.angles()
print("-----------------")
print(f"a = {a:.6f} Å, b = {b:.6f} Å, c = {c:.6f} Å")
print(f"α = {alpha:.4f}°, β = {beta:.4f}°, γ = {gamma:.4f}°")
# Display unit cell volume
volume = atoms_opt2.get_volume()
print(f" * unit cell volume: {volume:.4f} Å³")
print("-----------------")

print("=4= Begin calculating the phonons at the Gamma point！")

ph = Phonons(atoms_opt2, calc, supercell=(1,1,1), delta=0.01)
ph.clean()
# Perform displacement calculations (calculate the force on each atom)
ph.run()

# Read the results and construct a dynamic matrix.
ph.read(acoustic=True)    # Consider acoustic support correction
ph.clean()
```

```
q_point = [[0, 0, 0]]
# unit: eV
frequencies = ph.band_structure(q_point,verbose=False)

omega_eV = frequencies[0]

frequencies_cm = omega_eV * 8065.544

#Print the Gamma point phonon frequencies (unit: THz, positive values indicate
stability, negative values indicate imaginary frequencies indicating instability).
print("Gamma point phonon frequency (cm-1):")
for i, freq in enumerate(frequencies_cm):
      print(f"mode {i+1: 3d}: {freq:16.2f} cm-1")

print("----------------------------------------")
# Phonon calculator

N = 3

print(f"=5= Start of phonon computation{N: 2d} x {N: 2d} x {N: 2d}")
ph2 = Phonons(atoms_opt2, calc, supercell=(N, N, N), delta=0.01)
ph2.run()

# Read forces and assemble the dynamical matrix
ph2.read(acoustic=True)

ph2.clean()

# The webpage defines point K; select a closed loop.
# Check https://ase-lib.org/ase/dft/bztable.html
#
path = atoms_opt2.cell.bandpath(npoints=100)

bs= ph2.get_band_structure(path, verbose=False)

energies_ev = bs.energies[0]
```

```
energies_cm = energies_ev * 8065.544

fig = plt.figure(figsize=(8, 6))
ax = fig.add_axes([0.12, 0.07, 0.67, 0.85])

x_coords, label_x_coords, label_names = bs.path.get_linear_kpoint_axis()
ax.plot(x_coords, energies_cm, color='blue')
labels = [name if name != 'G' else r'$\Gamma$' for name in label_names]
plt.xticks(label_x_coords, labels)

plt.xlim(x_coords[0], x_coords[-1])

plt.ylim(energies_cm.min() - 50, energies_cm.max() + 50)    # Adjust the range
appropriately

plt.axhline(0, color='k', ls='--', lw=0.5)    # The zero-frequency line is useful for
observing imaginary frequencies.

plt.xlabel('Wave vector')
plt.ylabel('Frequency (cm⁻¹)')
plt.title('Phonon Band Structure')

# Add vertical lines to separate high symmetry points
for xc in label_x_coords[1:-1]:
        plt.axvline(xc, color='gray', ls='--', lw=0.8)



dos = ph2.get_dos(kpts=(20, 20, 20),verbose=False).sample_grid(npts=100, width=1e-3)

## Plot the band structure and DOS:
#import matplotlib.pyplot as plt    # noqa

#fig = plt.figure(figsize=(7, 4))
#ax = fig.add_axes([0.12, 0.07, 0.67, 0.85])

#emax = 0.035
#bs.plot(ax=ax, emin=0.0, emax=emax)
```

```
dosax = fig.add_axes([0.8, 0.07, 0.17, 0.85])
dosax.fill_between(
        dos.get_weights(),
        dos.get_energies()* 8065.544,
        y2=0,
        color='grey',
        edgecolor='k',
        lw=1,
)

dosax.set_ylim(energies_cm.min() - 50, energies_cm.max() + 50)
dosax.set_xlim(left=0)
dosax.set_yticks([])
dosax.set_xticks([])
dosax.set_xlabel('DOS', fontsize=12)

print("Output phonon band phonon.png\n")
plt.savefig('phonon.png')
```

References:

[1]. Petkov V, Trikalitis P N, Bozin E S, et al. Structure of $V_2O_5 \cdot nH_2O$ Xerogel Solved by the Atomic Pair Distribution Function Technique[J]. Journal of the American Chemical Society, 2002, 124(34): 10157-10162.