Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Exotic hexagonal NaCl atom-thin layer on methylammonium lead iodide substrates, new hints for perovskite solar cells from first-principles calculations.

Adriana Pecoraro,[a,b] Ana B. Muñoz-García,[a,b,*] Gennaro V. Sannino,[c,d] Paola Delli Veneri,[d] and Michele Pavone [c,b,*]

(a) *Department of Physics "E. Pancini", University of Naples Federico II, Napoli, Italy*

(b) *INSTM-GISEL, National Interuniversity Consortium of Materials Science and Technology (INSTM), Florence, Italy*

(c) *Department of Chemical Sciences, University of Naples Federico II, Napoli, Italy*

(d) *Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Portici (NA), Italy*

*Corresponding authors:

MP michele.pavone@unina.it; ABMG anabelen.munozgarcia@unina.it

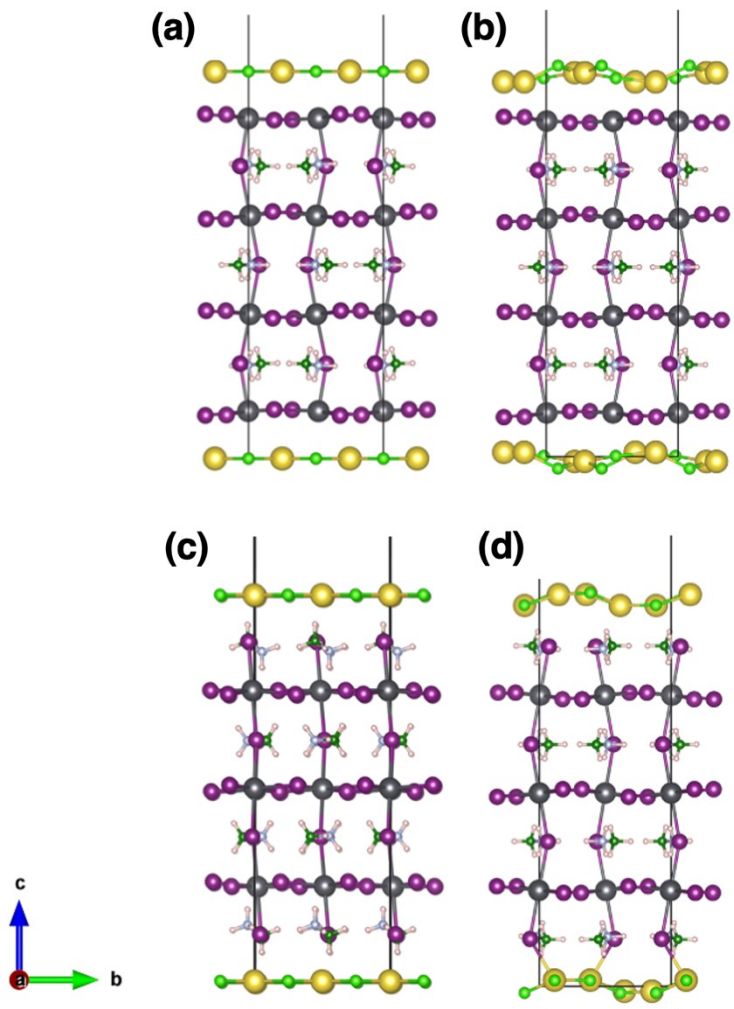

Figure S1: Theoretical models of the interface between a PbI_2- (upper panel) and a MAI- (lower panel) terminated MAPI substrate and a monolayer of NaCl. Figures (a,b) and (c,d) refer to structures before and after the geometrical optimization, respectively. Color labels of atomic spheres: Pb - dark gray; I - violet; C- green; N- light blue; H - light pink; Na - yellow; Cl - light green. Interfaces pertaining to stacking S1.

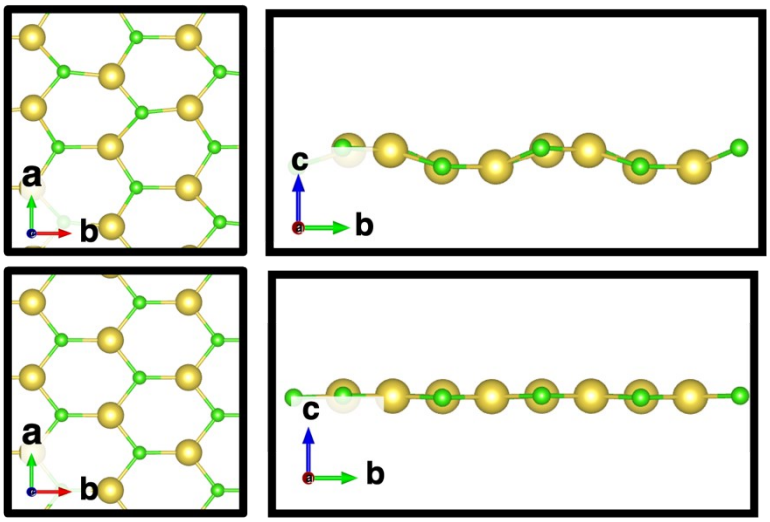

Figure S2: Top and side views off 1L of NaCl before (upper panel) and after (lower panel) the structural optimization without the perovskite substrate. The starting geometry pertain to the MAI interface in the S1 stacking.

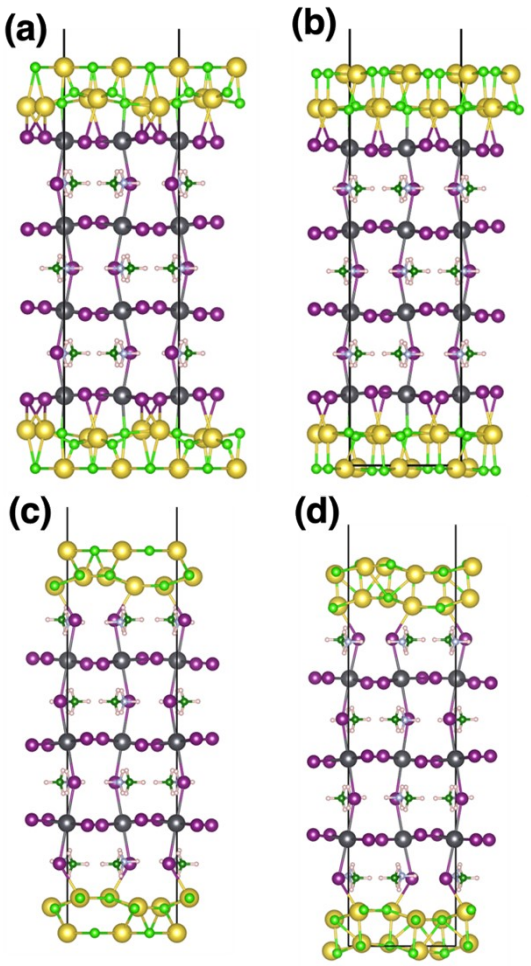

Figure S3: Theoretical models of the interface between a PbI_2- (upper panel) and a MAI- (lower panel) terminated MAPI substrate and a 2L of NaCl. Figures (a,b) and (c,d) refer to structures before and after the geometrical optimization, respectively. In both cases the second salt layer is added to the previously optimized interface.

Frequency analysis

To further asses the stability of the optimized MAPI/NaCl interfaces we calculate the vibrational frequencies of 14 and 12 atoms belonging to the interfaces of both the MAI and the PbI_2 terminations (Stacking S1), respectively. Atoms involved in the calculations are depicted in red in Figure S4. Frequency calculations have been performed in the Γ point by means of the finite differences method as implemented in the VASP software. Obtained frequency values are shown in Figure S5 for both the perovskite terminations. Notably, even expanding the set of involved atoms there are less than six imaginary modes as evident by Figure S6 where the set of atoms involved in the frequency calculation has been extended from 14 to 54 atoms for the MAI-terminated interface.

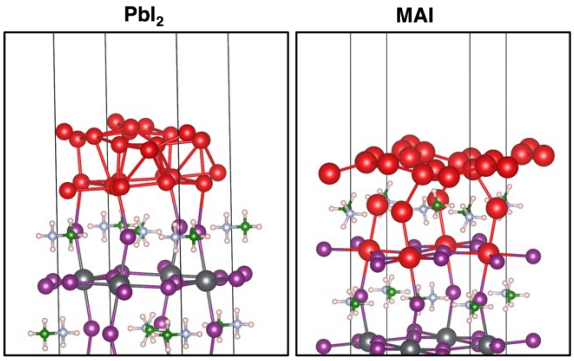

Figure S4: Optimized PbI_2 and MAI terminated MAPI/NaCl interfaces (Stacking S1). Color code: Pb - dark gray; I - violet; C- green; N- light blue; H - light pink. Atoms depicted in red (Na, Cl, Pb, I) are those for which vibrational frequencies have been calculated.

PbI_2

1	f	=	6.965619 THz	43.766277 2PiTHz	232.348044 cm-1	28.807496 meV
2	f	=	6.848913 THz	43.032990 2PiTHz	228.455143 cm-1	28.324838 meV
3	f	=	6.465182 THz	40.621937 2PiTHz	215.655257 cm-1	26.737854 meV
4	f	=	6.275159 THz	39.427984 2PiTHz	209.316752 cm-1	25.951979 meV
5	f	=	5.633638 THz	35.397193 2PiTHz	187.917938 cm-1	23.298863 meV
6	f	=	5.385408 THz	33.837516 2PiTHz	179.637865 cm-1	22.272265 meV
7	f	=	4.236759 THz	26.620340 2PiTHz	141.323054 cm-1	17.521832 meV
8	f	=	4.139197 THz	26.007343 2PiTHz	138.068753 cm-1	17.118350 meV
9	f	=	3.841686 THz	24.138027 2PiTHz	128.144856 cm-1	15.887943 meV
10	f	=	3.510993 THz	22.060219 2PiTHz	117.114115 cm-1	14.520305 meV
11	f	=	3.391049 THz	21.306587 2PiTHz	113.113202 cm-1	14.024255 meV
12	f	=	3.134593 THz	19.695229 2PiTHz	104.558765 cm-1	12.963639 meV
13	f	=	3.068875 THz	19.282308 2PiTHz	102.366636 cm-1	12.691850 meV
14	f	=	2.908492 THz	18.274593 2PiTHz	97.016841 cm-1	12.028560 meV
15	f	=	2.830267 THz	17.783093 2PiTHz	94.407549 cm-1	11.705048 meV
16	f	=	2.803226 THz	17.613186 2PiTHz	93.505540 cm-1	11.593214 meV
17	f	=	2.499383 THz	15.704084 2PiTHz	83.370427 cm-1	10.336619 meV
18	f	=	2.361676 THz	14.838851 2PiTHz	78.777046 cm-1	9.767112 meV
19	f	=	2.294928 THz	14.419455 2PiTHz	76.550542 cm-1	9.491061 meV
20	f	=	2.181855 THz	13.708999 2PiTHz	72.778844 cm-1	9.023430 meV
21	f	=	2.122381 THz	13.335311 2PiTHz	70.794995 cm-1	8.777464 meV
22	f	=	2.103106 THz	13.214202 2PiTHz	70.152046 cm-1	8.697748 meV
23	f	=	2.061108 THz	12.950324 2PiTHz	68.751162 cm-1	8.524061 meV
24	f	=	2.011745 THz	12.640168 2PiTHz	67.104594 cm-1	8.319912 meV
25	f	=	1.970231 THz	12.379324 2PiTHz	65.719817 cm-1	8.148222 meV
26	f	=	1.833349 THz	11.519273 2PiTHz	61.153949 cm-1	7.582126 meV
27	f	=	1.813874 THz	11.396907 2PiTHz	60.504327 cm-1	7.501583 meV
28	f	=	1.737778 THz	10.918788 2PiTHz	57.966026 cm-1	7.186874 meV
29	f	=	1.583770 THz	9.951121 2PiTHz	52.828883 cm-1	6.549949 meV
30	f	=	1.550279 THz	9.740693 2PiTHz	51.711756 cm-1	6.411443 meV
31	f	=	1.537318 THz	9.659254 2PiTHz	51.279410 cm-1	6.357839 meV
32	f	=	1.457896 THz	9.160233 2PiTHz	48.630185 cm-1	6.029377 meV
33	f	=	1.309483 THz	8.227722 2PiTHz	43.679637 cm-1	5.415587 meV
34	f	=	1.239031 THz	7.785061 2PiTHz	41.329622 cm-1	5.124222 meV
35	f	=	1.090620 THz	6.852569 2PiTHz	36.379172 cm-1	4.510444 meV
36	f	=	0.946890 THz	5.949487 2PiTHz	31.584859 cm-1	3.916025 meV
37	f	=	0.893337 THz	5.613004 2PiTHz	29.798523 cm-1	3.694547 meV
38	f	=	0.797649 THz	5.011779 2PiTHz	26.606718 cm-1	3.298814 meV
39	f	=	0.582864 THz	3.662245 2PiTHz	19.442263 cm-1	2.410534 meV
40	f	=	0.502463 THz	3.157067 2PiTHz	16.760358 cm-1	2.078020 meV
41	f	=	0.443074 THz	2.783916 2PiTHz	14.779355 cm-1	1.832407 meV
42	f/i	=	0.164681 THz	1.034721 2PiTHz	5.493164 cm-1	0.681066 meV

MAI

1	f	=	6.103491 THz	38.349365 2PiTHz	203.590537 cm-1	25.242019 meV
2	f	=	6.074264 THz	38.165724 2PiTHz	202.615619 cm-1	25.121144 meV
3	f	=	5.540621 THz	34.812751 2PiTHz	184.815233 cm-1	22.914177 meV
4	f	=	5.530574 THz	34.749618 2PiTHz	184.480069 cm-1	22.872622 meV
5	f	=	5.295665 THz	33.273642 2PiTHz	176.644349 cm-1	21.901116 meV
6	f	=	5.101685 THz	32.054835 2PiTHz	170.173901 cm-1	21.098882 meV
7	f	=	4.735102 THz	29.751522 2PiTHz	157.945987 cm-1	19.582814 meV
8	f	=	4.590590 THz	28.843528 2PiTHz	153.125599 cm-1	18.985161 meV
9	f	=	4.301553 THz	27.027452 2PiTHz	143.484344 cm-1	17.789798 meV
10	f	=	4.057749 THz	25.495588 2PiTHz	135.351928 cm-1	16.781506 meV
11	f	=	3.754862 THz	23.592492 2PiTHz	125.248704 cm-1	15.528866 meV
12	f	=	3.261763 THz	20.494259 2PiTHz	108.800687 cm-1	13.489571 meV
13	f	=	3.183833 THz	20.004612 2PiTHz	106.201228 cm-1	13.167279 meV
14	f	=	3.150716 THz	19.796532 2PiTHz	105.096569 cm-1	13.030319 meV
15	f	=	2.982617 THz	18.740335 2PiTHz	99.489391 cm-1	12.335117 meV
16	f	=	2.780042 THz	17.467519 2PiTHz	92.732214 cm-1	11.497333 meV
17	f	=	2.655213 THz	16.683198 2PiTHz	88.568382 cm-1	10.981084 meV
18	f	=	2.561772 THz	16.096090 2PiTHz	85.451525 cm-1	10.594643 meV
19	f	=	2.513397 THz	15.792140 2PiTHz	83.837900 cm-1	10.394579 meV
20	f	=	2.468866 THz	15.512345 2PiTHz	82.352517 cm-1	10.210414 meV
21	f	=	2.437605 THz	15.315923 2PiTHz	81.309746 cm-1	10.081127 meV
22	f	=	2.419019 THz	15.199142 2PiTHz	80.689770 cm-1	10.004260 meV
23	f	=	2.069266 THz	13.001582 2PiTHz	69.023284 cm-1	8.557800 meV
24	f	=	1.808840 THz	11.365274 2PiTHz	60.336391 cm-1	7.480762 meV
25	f	=	1.701638 THz	10.691705 2PiTHz	56.760523 cm-1	7.037411 meV
26	f	=	1.666180 THz	10.468920 2PiTHz	55.577795 cm-1	6.890771 meV
27	f	=	1.617990 THz	10.166134 2PiTHz	53.970350 cm-1	6.691473 meV
28	f	=	1.583318 THz	9.948280 2PiTHz	52.813800 cm-1	6.548079 meV
29	f	=	1.499630 THz	9.422452 2PiTHz	50.022262 cm-1	6.201972 meV
30	f	=	1.468642 THz	9.227751 2PiTHz	48.988628 cm-1	6.073818 meV
31	f	=	1.410288 THz	8.861101 2PiTHz	47.042144 cm-1	5.832485 meV
32	f	=	1.330860 THz	8.362040 2PiTHz	44.392708 cm-1	5.503996 meV
33	f	=	1.223323 THz	7.686364 2PiTHz	40.805656 cm-1	5.059258 meV
34	f	=	1.129274 THz	7.095440 2PiTHz	37.668537 cm-1	4.670305 meV
35	f	=	0.824376 THz	5.179706 2PiTHz	27.498215 cm-1	3.409345 meV
36	f	=	0.668036 THz	4.197393 2PiTHz	22.283276 cm-1	2.762775 meV

Figure S5: Vibrational frequencies pertaining to atoms of the PbI_2 and MAI terminated interfaces depicted in red in figure S4.

MAI

1	f	=	94.889437 THz	596.207917 2PiTHz	3165.170826 cm-1	392.431308 meV	53	f	=	37.486041 THz	235.029089 2PiTHz	1247.731193 cm-1	154.699087 meV	114	f	=	2.807350 THz	17.639101 2PiTHz	93.643116 cm-1	11.610271 meV
2	f	=	94.716392 THz	595.120642 2PiTHz	3159.398659 cm-1	391.715651 meV	54	f	=	37.362757 THz	234.757125 2PiTHz	1246.287379 cm-1	154.519997 meV	115	f	=	2.743833 THz	17.240811 2PiTHz	91.524416 cm-1	11.347585 meV
3	f	=	94.199832 THz	591.875003 2PiTHz	3142.168091 cm-1	389.579332 meV	55	f	=	37.285984 THz	234.274243 2PiTHz	1243.723840 cm-1	154.202159 meV	116	f	=	2.722845 THz	17.108137 2PiTHz	90.824315 cm-1	11.260784 meV
4	f	=	94.180910 THz	591.756107 2PiTHz	3141.536892 cm-1	389.501073 meV	56	f	=	37.264989 THz	234.142829 2PiTHz	1243.026183 cm-1	154.115660 meV	117	f	=	2.691301 THz	16.909946 2PiTHz	89.772150 cm-1	11.130332 meV
5	f	=	93.674977 THz	588.577237 2PiTHz	3124.660786 cm-1	387.408702 meV	57	f	=	29.606326 THz	186.022034 2PiTHz	987.560712 cm-1	122.441967 meV	118	f	=	2.646481 THz	16.628333 2PiTHz	88.277114 cm-1	10.944971 meV
6	f	=	93.660954 THz	588.489132 2PiTHz	3124.193052 cm-1	387.350710 meV	58	f	=	29.584459 THz	185.884640 2PiTHz	986.831312 cm-1	122.351533 meV	119	f	=	2.598340 THz	16.325849 2PiTHz	86.671275 cm-1	10.745872 meV
7	f	=	93.551910 THz	587.803984 2PiTHz	3120.555716 cm-1	386.899738 meV	59	f	=	29.548838 THz	185.660822 2PiTHz	985.643098 cm-1	122.204213 meV	120	f	=	2.553745 THz	16.045654 2PiTHz	85.183768 cm-1	10.561445 meV
8	f	=	93.540092 THz	587.729733 2PiTHz	3120.161527 cm-1	386.850865 meV	60	f	=	27.898302 THz	175.290203 2PiTHz	930.587168 cm-1	115.378146 meV	121	f	=	2.543172 THz	15.979222 2PiTHz	84.831090 cm-1	10.517718 meV
9	f	=	93.404232 THz	586.876098 2PiTHz	3115.629716 cm-1	386.288991 meV	61	f	=	27.869514 THz	175.109322 2PiTHz	929.626900 cm-1	115.259087 meV	122	f	=	2.531767 THz	15.907560 2PiTHz	84.450648 cm-1	10.470550 meV
10	f	=	93.375875 THz	586.697923 2PiTHz	3114.683818 cm-1	386.171715 meV	62	f	=	27.455382 THz	172.507256 2PiTHz	915.812954 cm-1	113.546376 meV	123	f	=	2.497196 THz	15.690343 2PiTHz	83.297479 cm-1	10.327575 meV
11	f	=	93.131485 THz	585.162380 2PiTHz	3106.531867 cm-1	385.161002 meV	63	f	=	27.436157 THz	172.386460 2PiTHz	915.171669 cm-1	113.466867 meV	124	f	=	2.489154 THz	15.137161 2PiTHz	80.360724 cm-1	9.963464 meV
12	f	=	93.090600 THz	584.905489 2PiTHz	3105.168073 cm-1	384.991913 meV	64	f	=	27.405593 THz	172.194417 2PiTHz	914.152142 cm-1	113.340461 meV	125	f	=	2.399864 THz	15.078789 2PiTHz	80.050837 cm-1	9.925042 meV
13	f	=	92.841256 THz	583.338815 2PiTHz	3096.850857 cm-1	383.960709 meV	65	f	=	27.334916 THz	171.750345 2PiTHz	911.794637 cm-1	113.048168 meV	126	f	=	2.301301 THz	14.459502 2PiTHz	76.763145 cm-1	9.517420 meV
14	f	=	92.809907 THz	583.141843 2PiTHz	3095.805166 cm-1	383.831060 meV	66	f	=	27.334916 THz	171.750345 2PiTHz	911.794637 cm-1	113.048168 meV	127	f	=	2.290268 THz	14.390181 2PiTHz	76.395128 cm-1	9.471792 meV
15	f	=	92.430206 THz	580.756110 2PiTHz	3083.139699 cm-1	382.260741 meV	67	f	=	26.865976 THz	168.803909 2PiTHz	896.152487 cm-1	111.100788 meV	128	f	=	2.238957 THz	14.067783 2PiTHz	74.683573 cm-1	9.259586 meV
16	f	=	92.346744 THz	580.231708 2PiTHz	3080.355731 cm-1	381.915573 meV	68	f	=	26.779375 THz	168.259778 2PiTHz	893.263783 cm-1	110.750634 meV	129	f	=	2.087111 THz	13.113705 2PiTHz	69.618524 cm-1	8.631600 meV
17	f	=	92.182803 THz	579.201636 2PiTHz	3074.887249 cm-1	381.237568 meV	69	f	=	13.391625 THz	84.142060 2PiTHz	446.696586 cm-1	55.383328 meV	130	f	=	1.899894 THz	11.937386 2PiTHz	63.373638 cm-1	7.857333 meV
18	f	=	92.109626 THz	578.741848 2PiTHz	3072.446386 cm-1	380.934929 meV	70	f	=	13.331067 THz	83.761563 2PiTHz	444.676587 cm-1	55.132880 meV	131	f	=	1.876321 THz	11.789270 2PiTHz	62.587315 cm-1	7.759841 meV
19	f	=	91.366169 THz	574.070570 2PiTHz	3047.647253 cm-1	377.860237 meV	71	f	=	11.413934 THz	71.715865 2PiTHz	380.727860 cm-1	47.204255 meV	132	f	=	1.728093 THz	10.857927 2PiTHz	57.642969 cm-1	7.146820 meV
20	f	=	91.184055 THz	572.926315 2PiTHz	3041.572590 cm-1	377.107075 meV	72	f	=	11.227287 THz	70.543128 2PiTHz	374.501988 cm-1	46.432345 meV	133	f	=	1.676511 THz	10.533827 2PiTHz	55.922371 cm-1	6.933493 meV
21	f	=	90.251697 THz	567.068135 2PiTHz	3010.472465 cm-1	373.251149 meV	73	f	=	6.701461 THz	42.106522 2PiTHz	223.536477 cm-1	27.715026 meV	134	f	=	1.648954 THz	10.360683 2PiTHz	55.003178 cm-1	6.819527 meV
22	f	=	90.215399 THz	566.840071 2PiTHz	3009.261709 cm-1	373.101035 meV	74	f	=	6.358100 THz	39.949119 2PiTHz	212.083370 cm-1	26.294996 meV	135	f	=	1.626693 THz	10.220814 2PiTHz	54.260638 cm-1	6.727464 meV
23	f	=	89.902159 THz	564.871925 2PiTHz	2998.813144 cm-1	371.805577 meV	75	f	=	6.103342 THz	38.348429 2PiTHz	203.585572 cm-1	25.241403 meV	136	f	=	1.595930 THz	10.027521 2PiTHz	53.234479 cm-1	6.600237 meV
24	f	=	89.844469 THz	564.509450 2PiTHz	2996.888820 cm-1	371.566991 meV	76	f	=	6.080288 THz	38.203576 2PiTHz	202.816567 cm-1	25.144958 meV	137	f	=	1.558025 THz	9.789359 2PiTHz	51.970113 cm-1	6.443475 meV
25	f	=	48.215875 THz	302.944250 2PiTHz	1608.281735 cm-1	199.401593 meV	77	f	=	6.063404 THz	38.097490 2PiTHz	202.253377 cm-1	25.076232 meV	138	f	=	1.485635 THz	9.334521 2PiTHz	49.555455 cm-1	6.144096 meV
26	f	=	48.178247 THz	302.712852 2PiTHz	1607.053280 cm-1	199.249284 meV	78	f	=	6.005817 THz	37.735660 2PiTHz	200.332480 cm-1	24.838071 meV	139	f	=	1.480767 THz	9.303931 2PiTHz	49.393057 cm-1	6.123961 meV
27	f	=	47.700675 THz	299.712179 2PiTHz	1591.123196 cm-1	197.274205 meV	79	f	=	5.881005 THz	36.448789 2PiTHz	193.580688 cm-1	23.991036 meV	140	f	=	1.458099 THz	9.142658 2PiTHz	48.536886 cm-1	6.017809 meV
28	f	=	47.634073 THz	299.293708 2PiTHz	1588.901600 cm-1	196.998762 meV	80	f	=	5.694656 THz	35.780578 2PiTHz	189.953268 cm-1	23.551212 meV	141	f	=	1.439297 THz	9.043373 2PiTHz	48.009795 cm-1	5.952458 meV
29	f	=	47.363445 THz	297.593301 2PiTHz	1579.874416 cm-1	195.879533 meV	81	f	=	5.674371 THz	35.653122 2PiTHz	189.276624 cm-1	23.467319 meV	142	f	=	1.322837 THz	8.311632 2PiTHz	44.125101 cm-1	5.470817 meV
30	f	=	47.302871 THz	297.212702 2PiTHz	1577.853876 cm-1	195.629018 meV	82	f	=	5.596244 THz	35.162238 2PiTHz	186.670598 cm-1	23.144213 meV	143	f	=	1.308422 THz	8.221061 2PiTHz	43.644274 cm-1	5.411202 meV
31	f	=	47.242543 THz	296.833649 2PiTHz	1575.841547 cm-1	195.379521 meV	83	f	=	5.392996 THz	33.885190 2PiTHz	179.890961 cm-1	22.303645 meV	144	f	=	1.279001 THz	8.036198 2PiTHz	42.662865 cm-1	5.289523 meV
32	f	=	47.159848 THz	296.314061 2PiTHz	1573.083140 cm-1	195.037522 meV	84	f	=	5.282132 THz	33.188613 2PiTHz	176.192944 cm-1	21.845149 meV	145	f	=	1.234338 THz	7.755577 2PiTHz	41.173095 cm-1	5.104815 meV
33	f	=	43.561366 THz	273.704134 2PiTHz	1453.050717 cm-1	180.155393 meV	85	f	=	5.273459 THz	33.134120 2PiTHz	175.903651 cm-1	21.809281 meV	146	f	=	1.170092 THz	7.351908 2PiTHz	39.030082 cm-1	4.839115 meV
34	f	=	43.528055 THz	273.494838 2PiTHz	1451.939598 cm-1	180.017632 meV	86	f	=	5.139130 THz	32.290186 2PiTHz	171.422918 cm-1	21.253741 meV	147	f	=	1.130372 THz	7.102338 2PiTHz	37.705156 cm-1	4.674845 meV
35	f	=	43.414048 THz	272.778508 2PiTHz	1448.136718 cm-1	179.546135 meV	87	f	=	5.063481 THz	31.814787 2PiTHz	168.899526 cm-1	20.940880 meV	148	f	=	1.108980 THz	6.967926 2PiTHz	36.991584 cm-1	4.586374 meV
36	f	=	43.391351 THz	272.635981 2PiTHz	1447.379639 cm-1	179.452269 meV	88	f	=	4.967188 THz	31.209760 2PiTHz	165.687539 cm-1	20.542644 meV	149	f	=	1.061360 THz	6.668721 2PiTHz	35.403154 cm-1	4.389433 meV
37	f	=	43.280610 THz	271.940896 2PiTHz	1443.685722 cm-1	178.994281 meV	89	f	=	4.948096 THz	31.044630 2PiTHz	164.810888 cm-1	20.433953 meV	150	f	=	1.028884 THz	6.464169 2PiTHz	34.317219 cm-1	4.254794 meV
38	f	=	43.259835 THz	271.806532 2PiTHz	1442.966036 cm-1	178.905052 meV	90	f	=	4.896326 THz	30.744527 2PiTHz	163.323867 cm-1	20.249586 meV	151	f	=	0.937158 THz	5.888339 2PiTHz	31.260233 cm-1	3.875776 meV
39	f	=	43.242377 THz	271.699868 2PiTHz	1442.410392 cm-1	178.836160 meV	91	f	=	4.714420 THz	29.621574 2PiTHz	157.256119 cm-1	19.497281 meV	152	f	=	0.870660 THz	5.470518 2PiTHz	29.042089 cm-1	3.600761 meV
40	f	=	43.203111 THz	271.453155 2PiTHz	1441.100634 cm-1	178.673771 meV	92	f	=	4.631112 THz	29.098138 2PiTHz	154.477278 cm-1	19.152748 meV	153	f	=	0.765144 THz	4.807543 2PiTHz	25.522464 cm-1	3.164383 meV
41	f	=	43.135075 THz	271.025668 2PiTHz	1438.831176 cm-1	178.392394 meV	93	f	=	4.519685 THz	28.397517 2PiTHz	150.757796 cm-1	18.691591 meV	154	f	=	0.719163 THz	4.518634 2PiTHz	23.988694 cm-1	2.974220 meV
42	f	=	43.118886 THz	270.923954 2PiTHz	1438.291190 cm-1	178.325444 meV	94	f	=	4.497589 THz	28.259185 2PiTHz	150.023418 cm-1	18.600540 meV	155	f	=	0.538393 THz	3.382820 2PiTHz	17.958842 cm-1	2.226613 meV
43	f	=	43.067252 THz	270.599527 2PiTHz	1436.568861 cm-1	178.111903 meV	95	f	=	4.400021 THz	27.646147 2PiTHz	146.768894 cm-1	18.197030 meV	156	f	=	0.513674 THz	3.227506 2PiTHz	17.134304 cm-1	2.124384 meV
44	f	=	43.032940 THz	270.383939 2PiTHz	1435.424338 cm-1	177.970000 meV	96	f	=	4.277311 THz	26.876138 2PiTHz	142.675737 cm-1	17.689543 meV	157	f	=	0.294987 THz	1.852957 2PiTHz	9.837046 cm-1	1.219639 meV
45	f	=	42.162634 THz	264.915640 2PiTHz	1406.394028 cm-1	174.370699 meV	97	f	=	4.041684 THz	25.394650 2PiTHz	134.816065 cm-1	16.715068 meV	158	f/i=		0.181583 THz	1.140918 2PiTHz	6.056950 cm-1	0.750966 meV
46	f	=	42.155441 THz	264.870450 2PiTHz	1406.154122 cm-1	174.340954 meV	98	f	=	4.026010 THz	25.296169 2PiTHz	134.293243 cm-1	16.650246 meV	159	f/i=		0.475981 THz	2.990679 2PiTHz	15.877028 cm-1	1.968501 meV
47	f	=	41.889487 THz	263.199412 2PiTHz	1397.282856 cm-1	173.241057 meV	99	f	=	3.972864 THz	24.957213 2PiTHz	132.493784 cm-1	16.427141 meV	160	f/i=		0.534768 THz	3.360049 2PiTHz	17.837953 cm-1	2.211625 meV
48	f	=	41.850534 THz	262.954660 2PiTHz	1395.983506 cm-1	173.079958 meV	100	f	=	3.798695 THz	23.867984 2PiTHz	126.710817 cm-1	15.710145 meV	161	f/i=		0.952477 THz	5.984591 2PiTHz	31.771219 cm-1	3.939130 meV
49	f	=	37.916861 THz	238.238665 2PiTHz	1264.770313 cm-1	156.811590 meV	101	f	=	3.742856 THz	23.517960 2PiTHz	124.848244 cm-1	15.479215 meV	162	f/i=		1.114171 THz	7.000541 2PiTHz	37.164734 cm-1	4.607841 meV
50	f	=	37.908677 THz	238.187245 2PiTHz	1264.497327 cm-1	156.777744 meV	102	f	=	3.661815 THz	23.007861 2PiTHz	122.144991 cm-1	15.144054 meV								
51	f	=	37.601123 THz	236.254825 2PiTHz	1254.238427 cm-1	155.505802 meV	103	f	=	3.530352 THz	22.181857 2PiTHz	117.759871 cm-1	14.600368 meV								
52	f	=	37.574662 THz	236.088562 2PiTHz	1253.355765 cm-1	155.396366 meV	104	f	=	3.391760 THz	21.311059 2PiTHz	113.136945 cm-1	14.027198 meV								
							105	f	=	3.332573 THz	20.939173 2PiTHz	111.162663 cm-1	13.782419 meV								
							106	f	=	3.296946 THz	20.715326 2PiTHz	109.974294 cm-1	13.635080 meV								
							107	f	=	3.211837 THz	20.180667 2PiTHz	107.135346 cm-1	13.283095 meV								
							108	f	=	3.172852 THz	19.935616 2PiTHz	105.834944 cm-1	13.121865 meV								
							109	f	=	3.056599 THz	19.205181 2PiTHz	101.957179 cm-1	12.641084 meV								
							110	f	=	3.010325 THz	18.914432 2PiTHz	100.413644 cm-1	12.449710 meV								
							111	f	=	2.975283 THz	18.694257 2PiTHz	99.244766 cm-1	12.304787 meV								
							112	f	=	2.902321 THz	18.235810 2PiTHz	96.810991 cm-1	12.003037 meV								
							113	f	=	2.838192 THz	17.782624 2PiTHz	94.405056 cm-1	11.704739 meV								

Figure S6: Vibrational frequencies pertaining to 54 atoms of MAI terminated interface.

We employ the Phonopy code to calculate the phonon band structure along the U-Γ-V Brillouin path, and the corresponding density of states. We use a 2x2x1 supercell model of the interface. Obtained results are shown in Figure S7. These additional analyses provide further confirmation of the stability of the examined structure and provides a comprehensive analysis of the phonon dispersion.

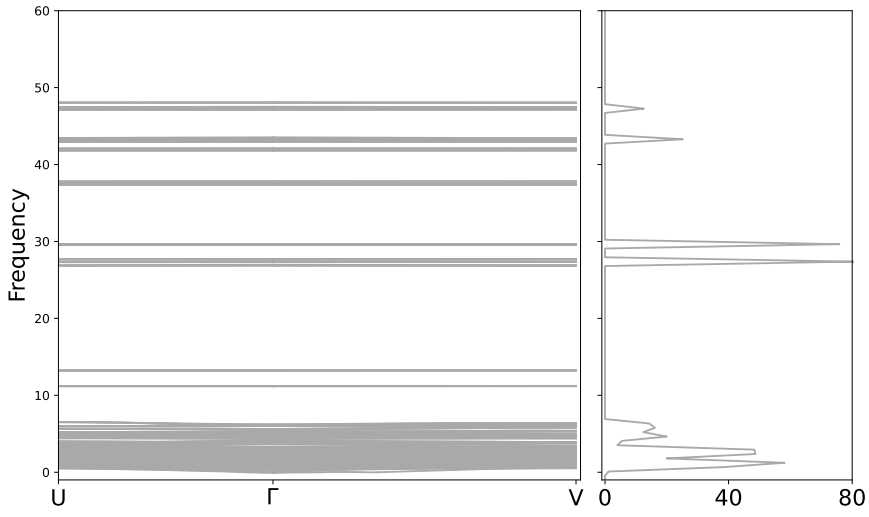

Figure S7: Phonon band structure and density of states for the MAI-terminated interface.