Supporting information (SI)

$Ag_2Mo_2O_7$: an oxide solid-state Ag^+ electrolyte

Weixin Yan[1], Dongmei Zhu[1], Zhaofeng Wang[1], Yunhao Xia[1], Dong-Yun Gui[2], Fa Luo[1], Chun-Hai Wang[1,3,*]

[1] State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi′an, Shaanxi 710072, China

[2] Institute of Functional Materials, College of Materials Science and Engineering, Xi′an University of Architecture and Technology, Xi′an, Shaanxi 710055, China

[3] School of Chemistry, The University of Sydney, Sydney NSW 2006, Australia

Table S1 Raman modes of $Ag_2Mo_2O_7$

	Experimental			Theoretical (DFT)	
mode	$f_{exp.}$ (cm^{-1})	$I_{exp.}$[a] (Arb.Unit)	FWHM (cm^{-1})	$f_{theo.}$ (cm^{-1})	$I_{theo.}$[a] (Arb.Unit)
$A_g^{(1)}$	-	-	-	32.00	0.00152
$A_g^{(2)}$	-	-	-	40.91	0.00266
$A_g^{(3)}$	-	-	-	46.49	0.00146
$A_g^{(4)}$	-	-	-	54.34	3.61E-4
$A_g^{(5)}$	-	-	-	74.93	0.00176
$A_g^{(6)}$	-	-	-	84.11	0.00169
$A_g^{(7)}$	101.9	0.0779	10.1	102.81	0.00192
$A_g^{(8)}$	116.4	0.0022	9.7	114.11	0.00352
$A_g^{(9)}$	-	-	-	140.20	0.00121
$A_g^{(10)}$	148.4	0.0135	16.0	142.71	0.00102
$A_g^{(11)}$	159.9	0.0759	12.2	154.86	0.00159
$A_g^{(12)}$	-	-	-	173.03	0.00401
$A_g^{(13)}$	187.8	0.0488	14.3	191.65	0.00311
$A_g^{(14)}$	-	-	-	213.04	0.00234
$A_g^{(15)}$	224.9	0.0488	16.4	224.52	0.00951
$A_g^{(16)}$	246.1	0.0385	13.3	242.64	0.00131
$A_g^{(17)}$	256.6	0.0508	16.5	262.72	0.02149
$A_g^{(18)}$	299.9	0.0355	15.1	303.12	0.02709
$A_g^{(19)}$	315.5	0.0574	14.0	304.17	0.03328
$A_g^{(20)}$	340.1	0.0111	14.3	328.57	0.01462
$A_g^{(21)}$	347.9	0.0481	10.3	333.57	0.01022
$A_g^{(22)}$	370.1	0.0060	14.4	347.75	0.01038
$A_g^{(23)}$	391.2	0.0069	14.2	372.88	0.00481
$A_g^{(24)}$	408.2	0	16.1	397.09	0.00661
$A_g^{(25)}$	470.2	0.0202	15.6	441.79	0.02214
$A_g^{(26)}$	501.0	0.0152	17.5	471.01	0.04616
$A_g^{(27)}$	602.6	0.0184	16.8	575.85	0.01423
$A_g^{(28)}$	664.2	0.1265	18.1	637.86	0.40601
$A_g^{(29)}$	732.0	0.0049	15.5	700.77	0.01021
$A_g^{(30)}$	826.7	0.1931	8.5	800.85	0.02425
$A_g^{(31)}$	833.8	0.3403	7.9	806.87	1.00000
$A_g^{(32)}$	886.1	0.1537	9.7	867.76	0.52889
$A_g^{(33)}$	915.7	1.0000	7.2	914.79	0.70337

[a]: Intensity are normalized

* Corresponding author, email: chwang81@gmail.com

Table S2 Eigenfrequency of infrared active vibrational modes of $Ag_2Mo_2O_7$ from the DFT calculations

No	Mode	f_{theo} (cm^{-1})	Intensity (km/mol)	No	Mode	f_{theo} (cm^{-1})	Intensity (km/mol)
1	$A_u^{(1)}$	38.75	1.07	16	$A_u^{(16)}$	306.14	5.12
2	$A_u^{(2)}$	54.05	1.67	17	$A_u^{(17)}$	324.64	3.89
3	$A_u^{(3)}$	60.89	2.68	18	$A_u^{(18)}$	335.17	10.81
4	$A_u^{(4)}$	91.17	0.79	19	$A_u^{(19)}$	351.41	18.44
5	$A_u^{(5)}$	98.38	1.23	20	$A_u^{(20)}$	361.13	8.88
6	$A_u^{(6)}$	113.83	1.82	21	$A_u^{(21)}$	386.71	16.57
7	$A_u^{(7)}$	126.84	1.21	22	$A_u^{(22)}$	398.45	10.38
8	$A_u^{(8)}$	141.51	0.99	23	$A_u^{(23)}$	437.13	1.33
9	$A_u^{(9)}$	168.75	1.23	24	$A_u^{(24)}$	535.02	141.23
10	$A_u^{(10)}$	195.51	0.22	25	$A_u^{(25)}$	649.70	33.87
11	$A_u^{(11)}$	202.21	0.66	26	$A_u^{(26)}$	697.18	52.98
12	$A_u^{(12)}$	213.20	22.62	27	$A_u^{(27)}$	795.65	40.13
13	$A_u^{(13)}$	242.56	1.87	28	$A_u^{(28)}$	817.39	12.07
14	$A_u^{(14)}$	254.11	7.58	29	$A_u^{(29)}$	865.84	24.67
15	$A_u^{(15)}$	291.78	25.84	30	$A_u^{(30)}$	905.88	27.04

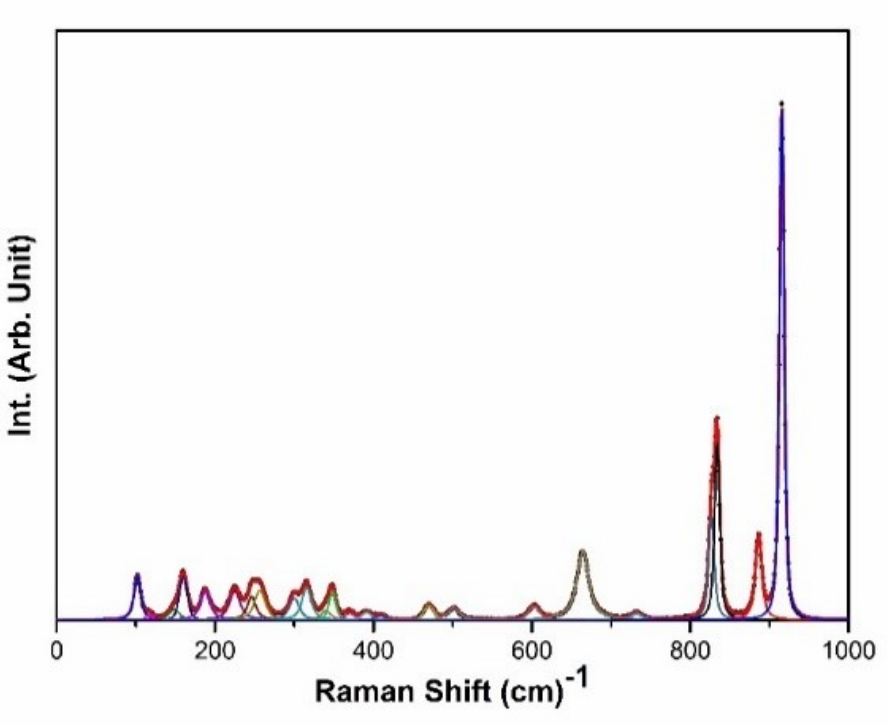

Fig. S1. Raman spectra of $Ag_2Mo_2O_7$ with fitted peaks.

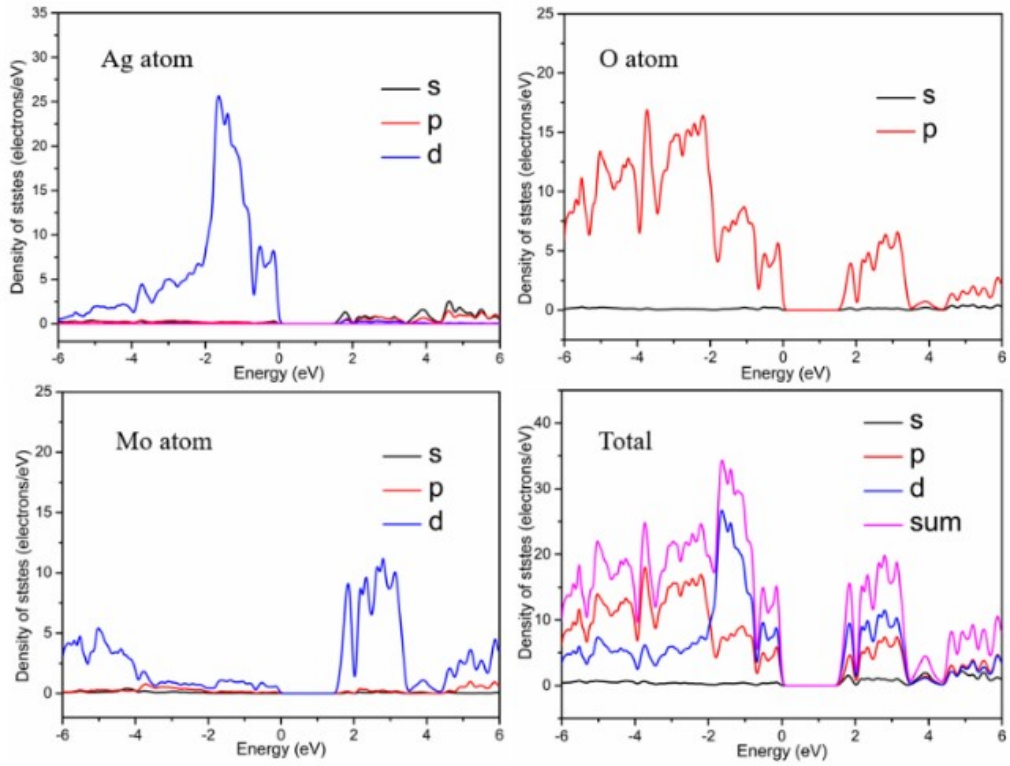

Fig. S2 Partial density of state (PDOS) of different atoms and total DOS in $Ag_2Mo_2O_7$. The Fermi level is set as E_{Femi} = 0 eV.

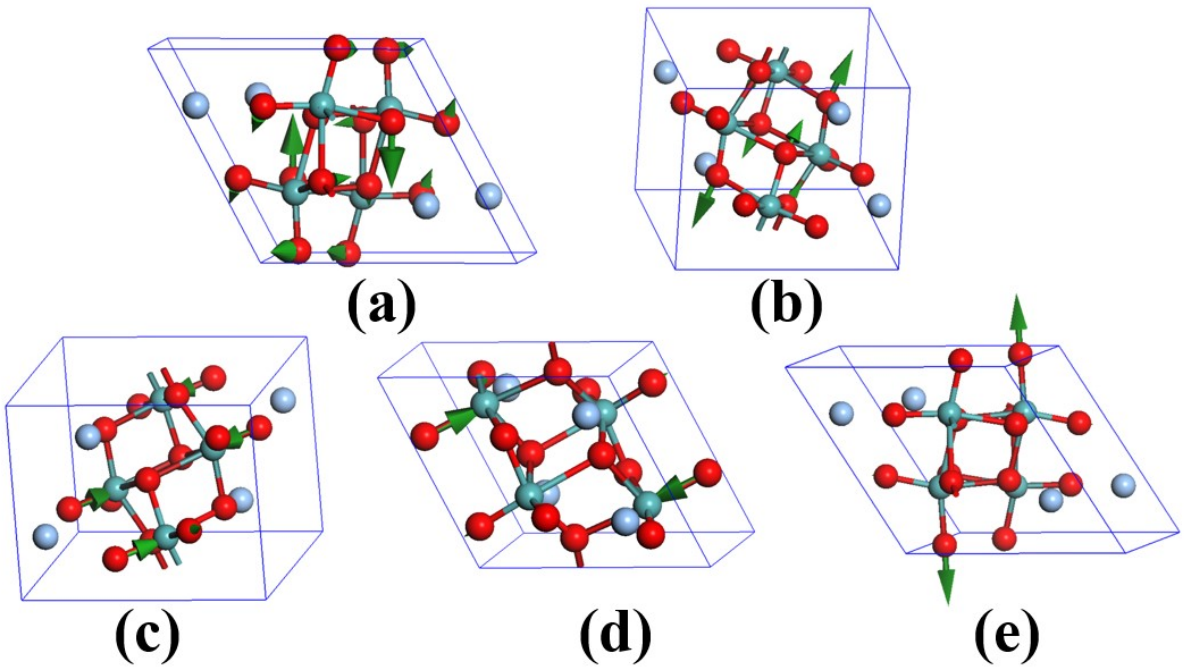

Fig. S3. The vibration detail (vector of atomic motions) of five Raman vibrational modes with high intensities (a) A_g (19) (304.17 cm^{-1}), (b) A_g (28) (637.86 cm^{-1}), (c) A_g (31) (806.87 cm^{-1}), (d) A_g (32) (867.76 cm^{-1}), (e) A_g (32) (914.79 cm^{-1}).

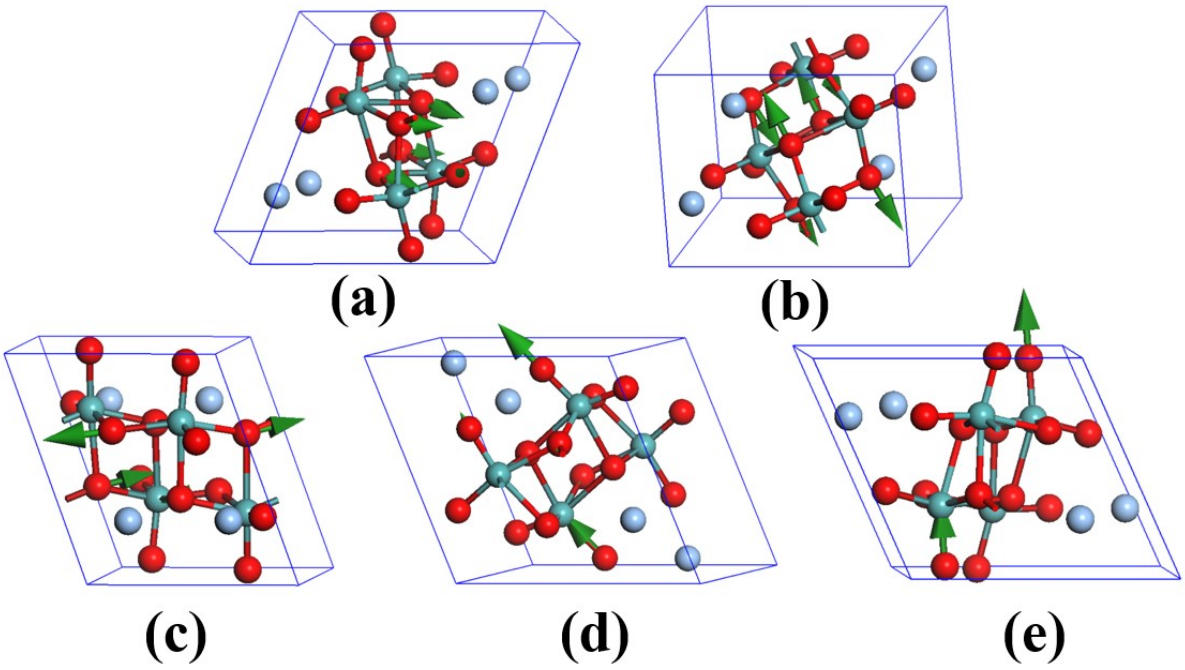

Fig. S4. The vibration detail (vector of atomic motions) of five IR vibrational modes with high intensities (a) $A_u^{(24)}$ (535.02 cm^{-1}), (b) $A_u^{(25)}$ (649.70 cm^{-1}), (c) $A_u^{(26)}$ (697.18 cm^{-1}), (d) $A_u^{(27)}$ (795.65 cm^{-1}), (e) $A_u^{(30)}$ (905.88 cm^{-1}).