

Supplementary material

Lattice Dynamics of KAgF₃ Perovskite, Unique 1D Antiferromagnet [†]

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† This work is dedicated to Josef Michl upon his 80th birthday

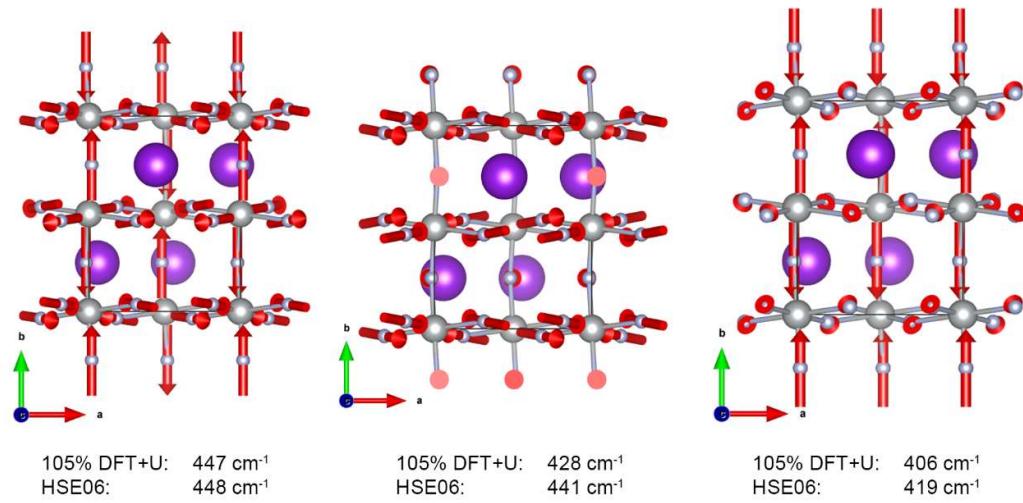
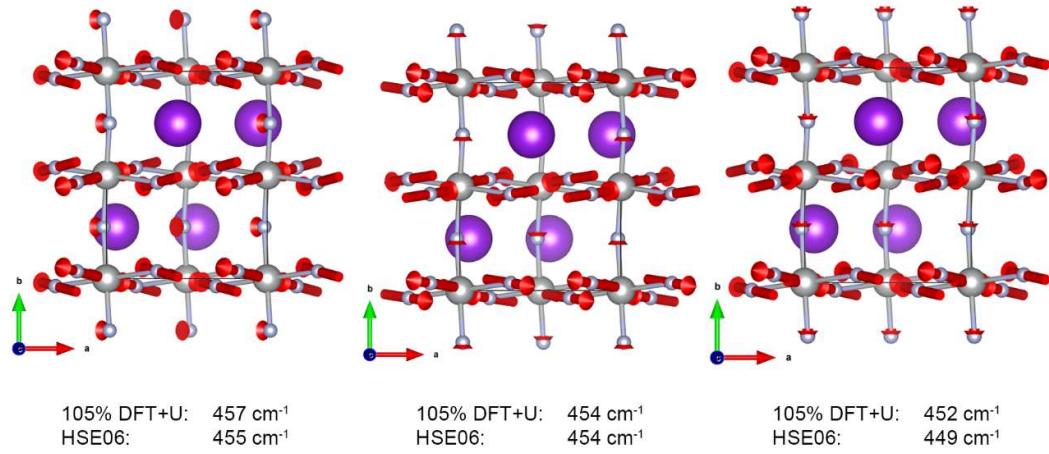
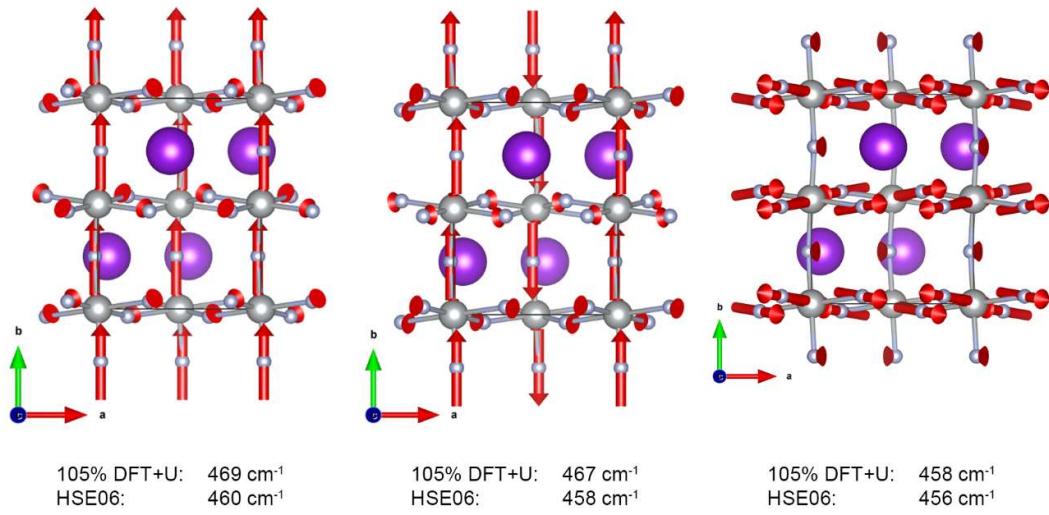
Abstract: Theoretical DFT calculations using GGA+U and HSE06 frameworks enabled vibrational mode assignment and partial (atomic) phonon DOS determination in KAgF₃ perovskite, a low-dimensional magnetic fluoroargentate(II). Twelve bands in the spectra of KAgF₃ were assigned to either IR active or Raman active modes, reaching very good correlation with experimental values ($R^2 > 0.997$). Low-temperature Raman measurements indicate that the intriguing spin-Peierls-like phase transition at 230 K is an order-disorder transition and it does not strongly impact the vibrational structure of the material.

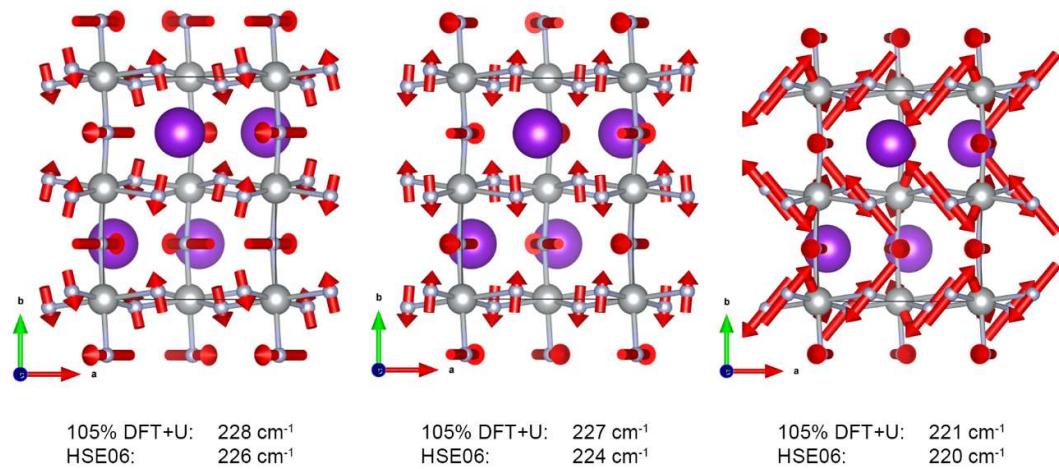
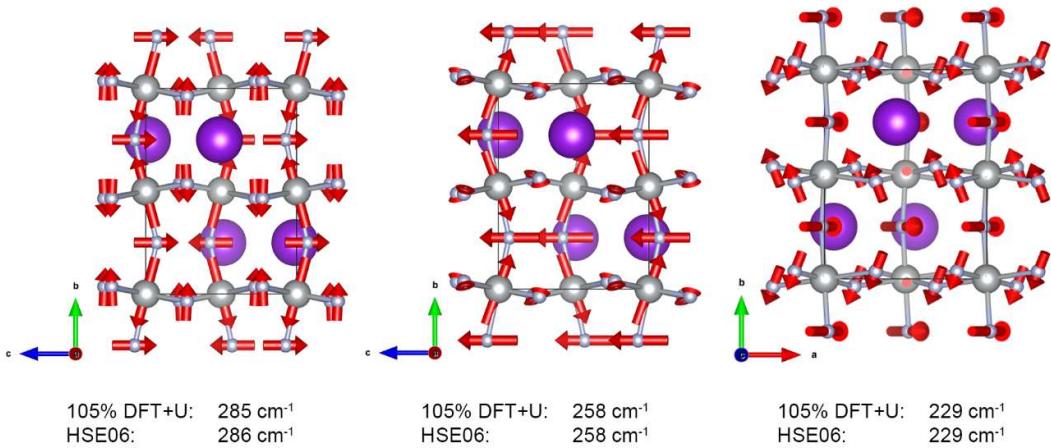
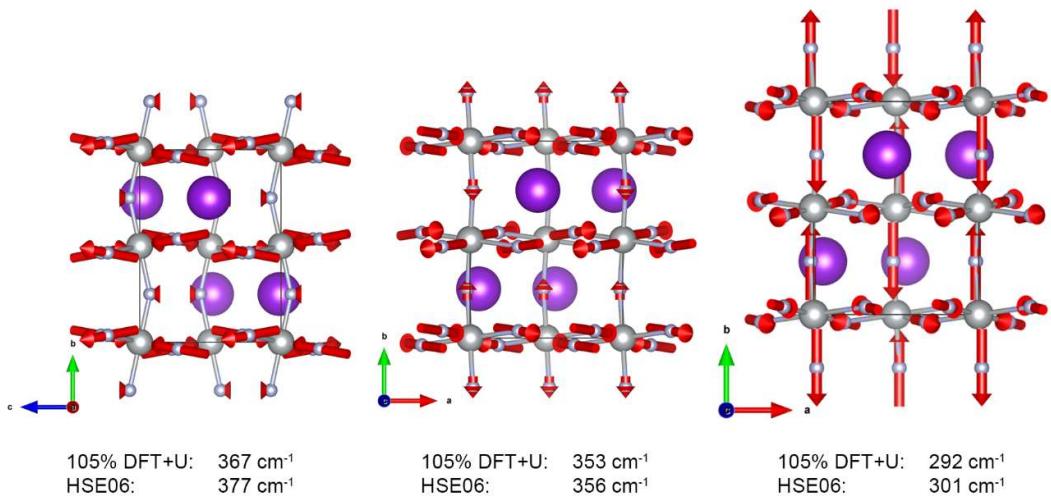
Keywords: theoretical modelling; silver fluorides; infrared spectra; Raman spectra; low dimensional materials

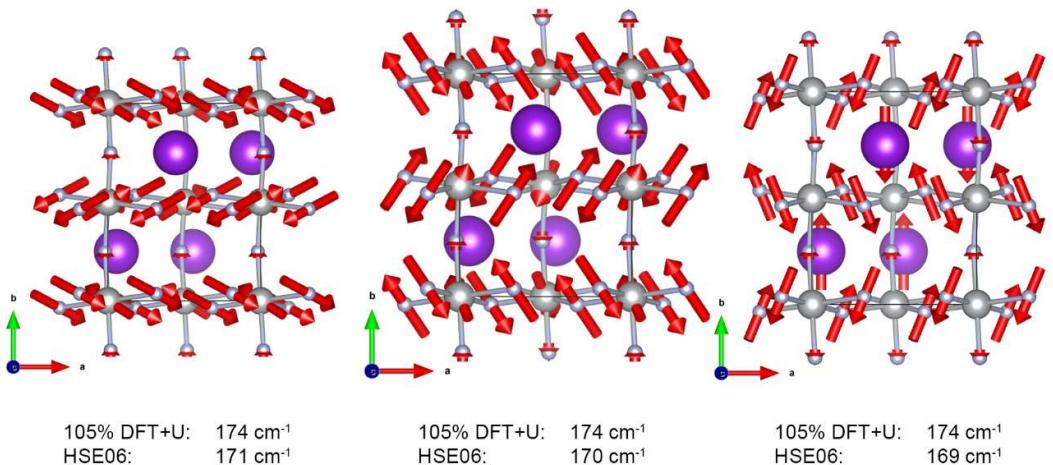
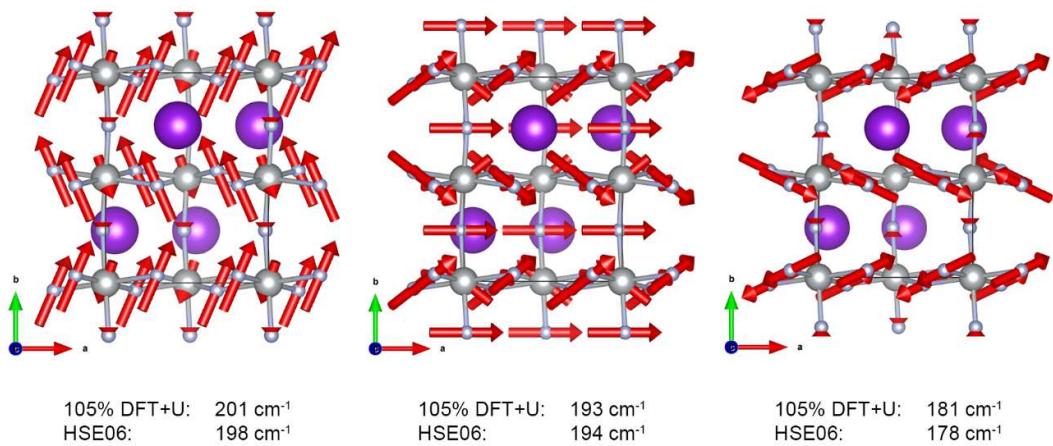
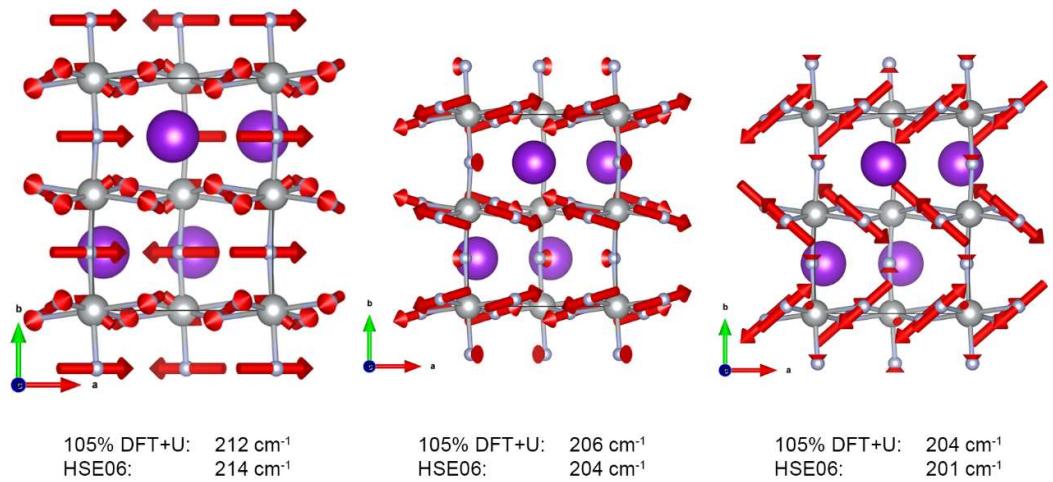
Table S1. List of all theoretically predicted normal modes (modes assigned to observable bands have been marked in bold fonts and grey background).

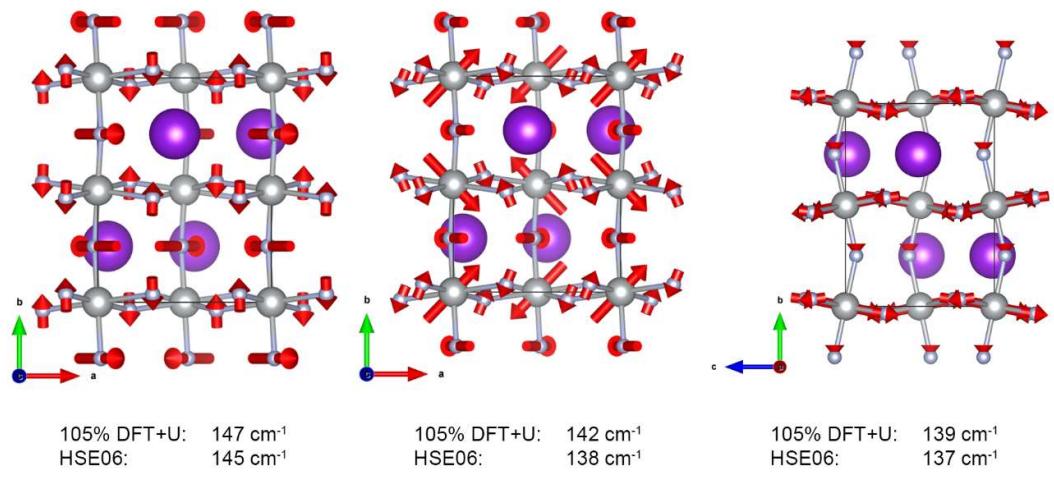
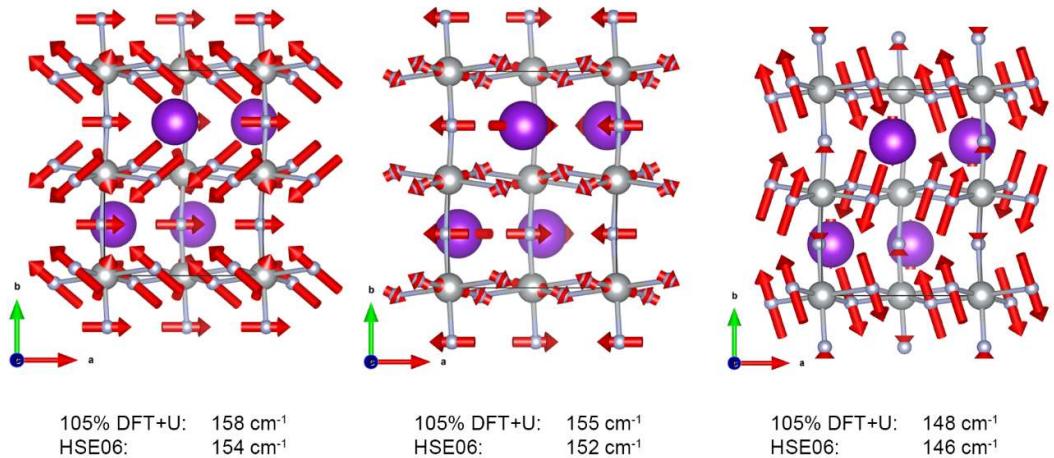
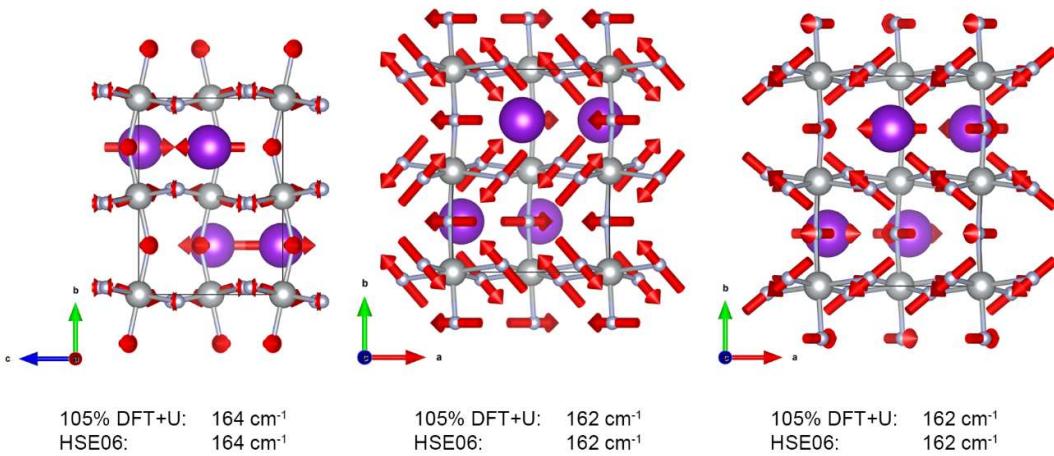
No.	105% DFT+U [cm ⁻¹]	HSE06 [cm ⁻¹]	Irreducible representation
1	469	460	B2u
2	467	458	Au
3	458	456	B1u
4	457	455	B3u
5	454	454	Au
6	452	449	B2u
7	447	448	B3g
8	428	441	B2g
9	406	419	B1g
10	367	377	Ag
11	353	356	B1g
12	292	301	B3g
13	285	286	B3u
14	258	258	B1u
15	229	229	B3u
16	228	226	B2g
17	227	224	Ag
18	221	220	B1u
19	212	214	B1u
20	206	204	B2g

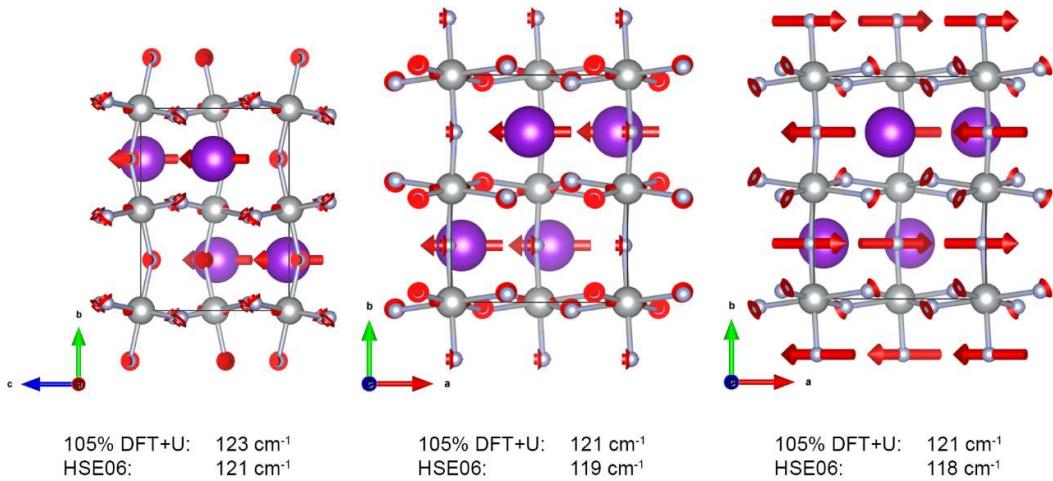
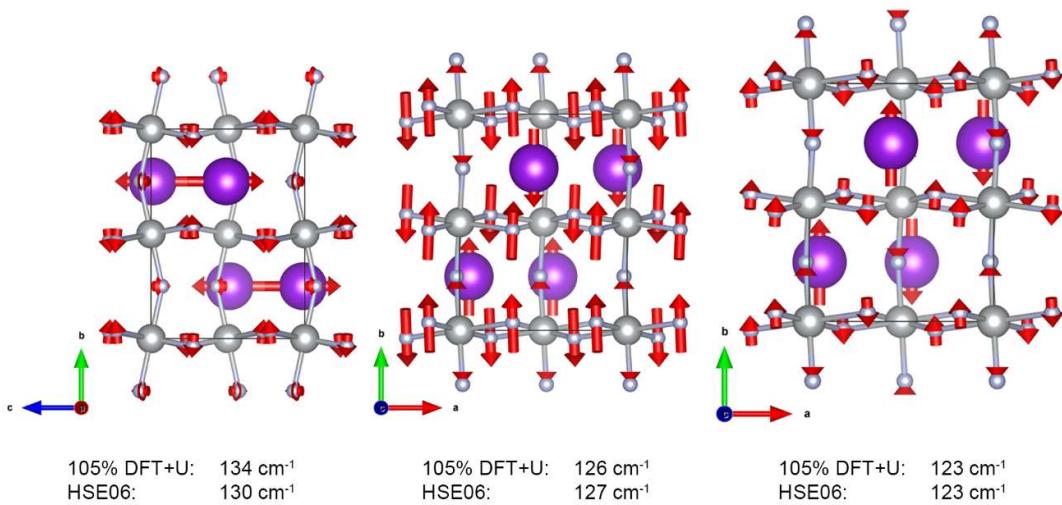
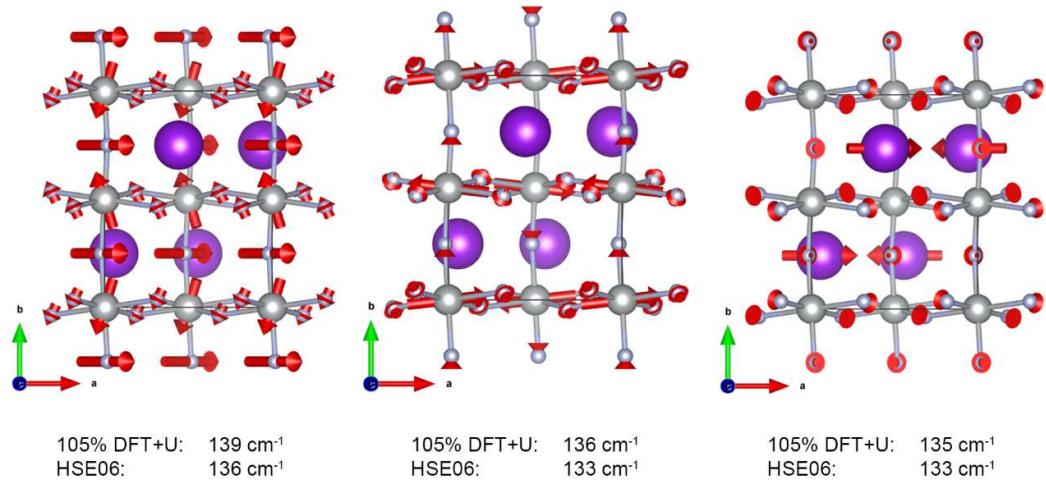
21	204	201	Au
22	202	198	B2u
23	193	194	B3u
24	181	178	B3g
25	174	171	B2u
26	174	170	B1g
27	173	169	Au
28	164	164	B3u
29	162	162	Ag
30	162	162	B1u
31	158	154	B3u
32	155	152	B1u
33	148	146	B3g
34	147	145	B2g
35	142	138	B1u
36	139	137	B3u
37	139	136	B2u
38	136	133	Au
39	135	133	B2g
40	134	130	Ag
41	126	127	B1g
42	123	123	B3g
43	123	121	Ag
44	121	119	B1u
45	121	118	B3u
46	108	105	B2u
47	104	103	Au
48	100	102	B2g
49	97	99	B1g
50	93	97	B2g
51	88	91	B1u
52	87	86	Ag
53	79	81	Ag
54	76	73	B3u
55	74	71	B2u
56	72	70	Au
57	64	61	Au
58	0	1	B3u
59	0	1	B2u
60	0	2	B1u

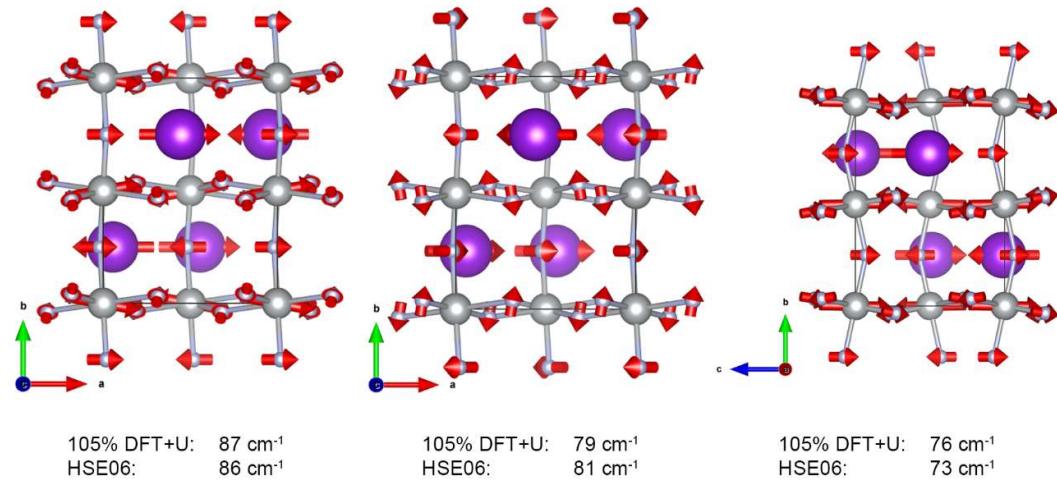
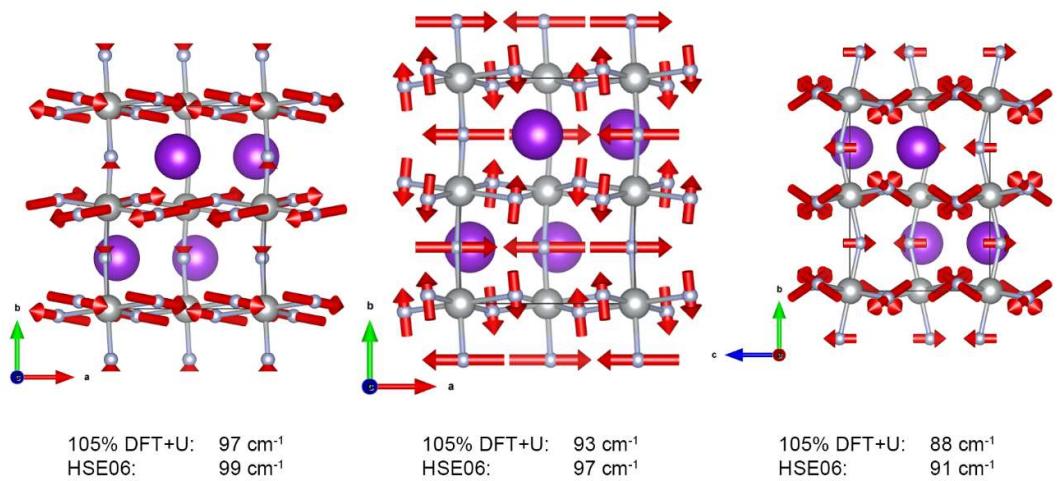
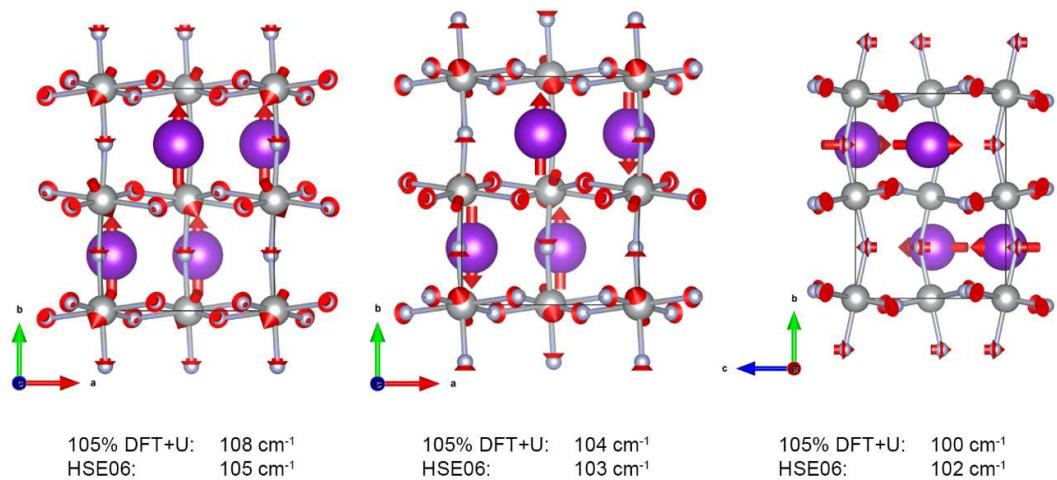












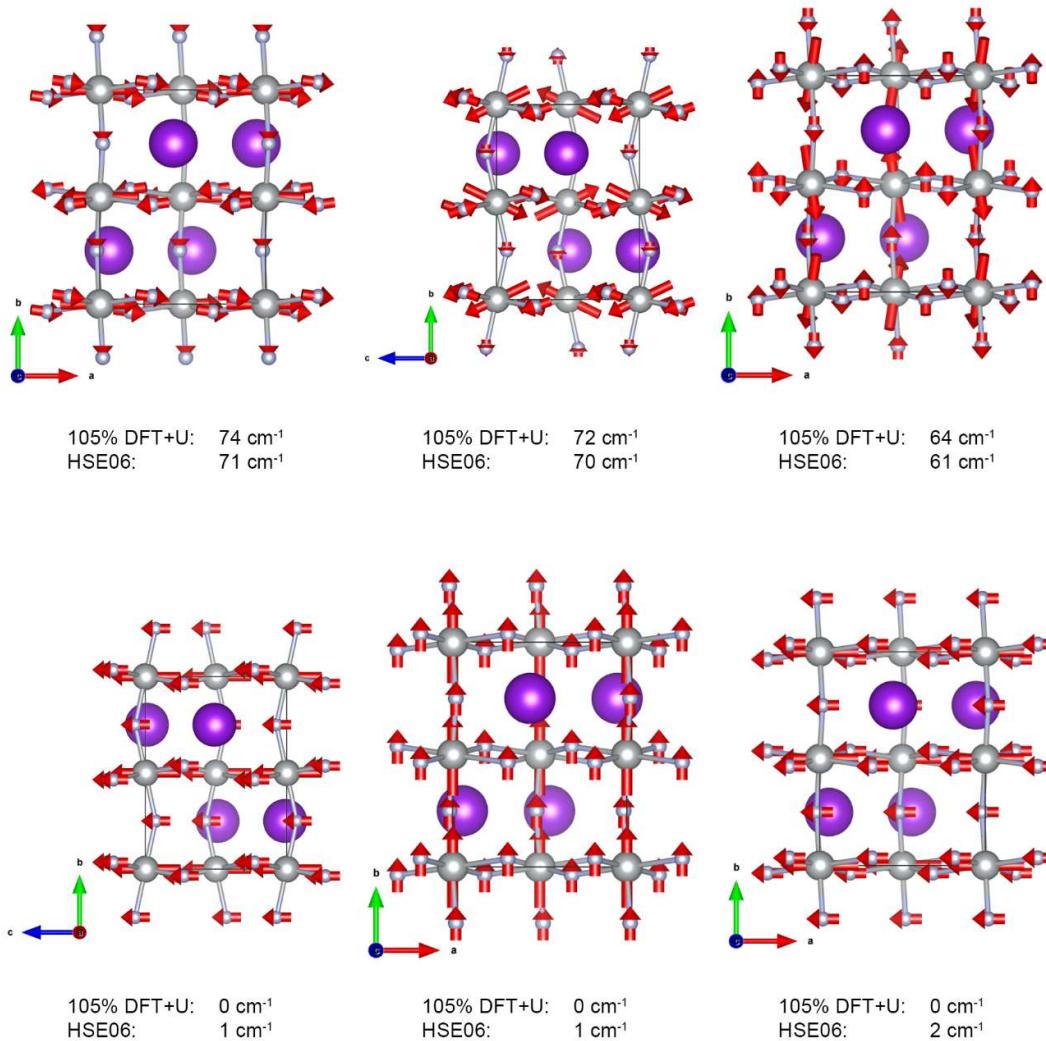


Figure 1. Visualization of theoretically predicted normal modes in order of decreasing wavenumbers.