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

Enhanced out-of-plane electromechanical response of Janus ZrSeO

Thi Hue Pham, Hamid Ullah, Aamir Shafique, Hye Jung Kim, and Young-Han Shin*

Multiscale Materials Modeling Laboratory, Department of Physics, University of Ulsan, Ulsan 44610, Republic of Korea

E-mail: hoponpop@ulsan.ac.kr

Table S1: The lattice parameters a and c (Å) and elastic coefficients (N/m), and binding energy E_b (eV/atom) of layered materials in monolayer and bulk structures.

	monolayer				bulk							
	a	C_{11}	C_{12}	E_b	a	c	c/a	C_{11}	C_{12}	C_{13}	C_{33}	E_b
ZrSeO	3.49	112	31	6.29	3.52	5.23	1.49	111	35	15	15	6.55
ZrSO	3.45	118	30	6.46	3.47	5.06	1.46	125	42	24	34	6.57
ZrSeS	3.73	71	15	5.43	3.72	6.05	1.62	71	15	5	20	5.51
HfSeO	3.45	122	30	6.53	3.47	5.29	1.52	123	35	14	17	6.63
HfSO	3.40	129	30	6.64	3.42	5.12	1.50	134	39	20	31	6.74
HfSeS	3.69	77	15	5.52	3.68	6.06	1.65	78	15	5	21	5.61
MoSeO	3.06	161	44	5.46	3.05	6.02	1.97	163	41	4	42	5.56
MoSO	3.00	176	51	5.58	3.00	5.92	1.97	178	49	3	37	5.66
MoSeS	3.26	119	28	4.71	3.23	6.89	2.13	125	30	7	37	4.96
WSeO	3.06	181	42	6.02	3.05	6.04	1.98	184	40	4	46	6.13
WSO	3.00	195	50	6.17	2.99	5.96	1.99	196	47	3	65	6.24
WSeS	3.25	131	27	5.23	3.23	6.90	2.14	136	26	5	35	5.48
C_2HF	2.57	247	25	5.50	2.56	4.79	1.87	251	28	4	28	5.82
HBNH	2.58	187	26	4.12	2.58	4.22	1.64	194	27	0.2	25	4.47
FBNF	2.66	189	35	5.39	2.66	5.79	2.18	182	32	0.7	28	5.47
HBNF	2.60	200	32	3.12	2.60	5.11	1.87	205	33	3	59	3.22

We examined the effect of vacuum thickness (h) on spontaneous polarization. The vacuum height h is defined as the difference between the supercell length normal to the layers and the thickness of the layers. The spontaneous polarization (P_3) were obtained with the increase in vacuum thickness of monolayer, bilayer, and trilayer ZrSeO to confirm their convergence which is shown in Fig. S1. If the length of c of monolayer, bilayer, and trilayer ZrSeO is higher than 22 Å, 28 Å, and 39 Å, respectively, the relative error is smaller than 0.1 %. In this work, we used $c = 30$ Å for monolayer and bilayer ZrSeO and $c = 40$ Å for trilayer ZrSeO.

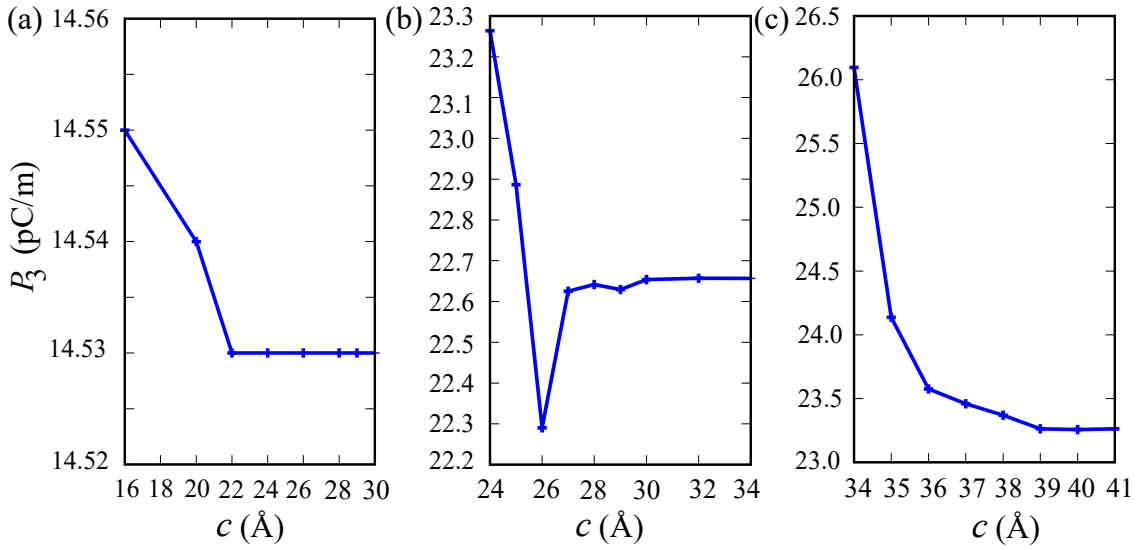

Figure S1: The spontaneous polarization per layer of (a) monolayer, (b) bilayer, and (c) trilayer ZrSeO with different c via the integration of the charge denensity method.

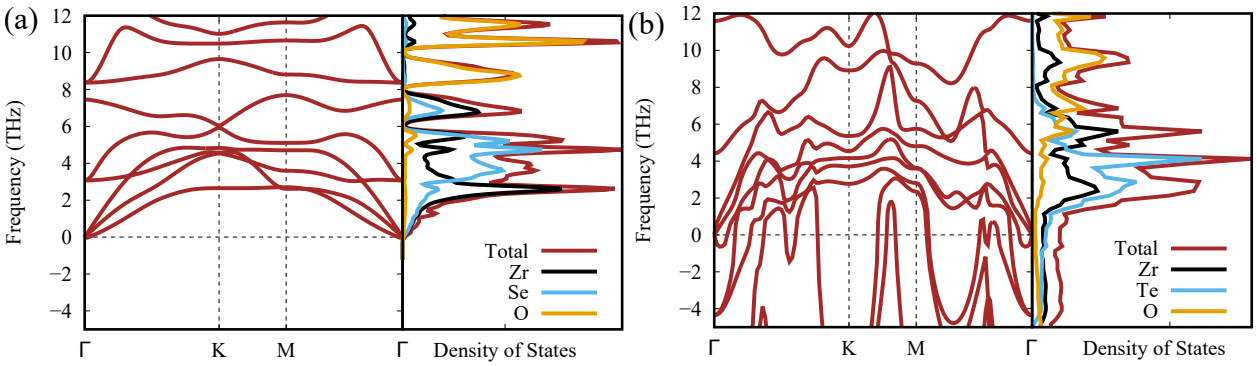

Figure S2: The phonon dispersion relations of (a) ZrSeO and (b) ZrTeO.

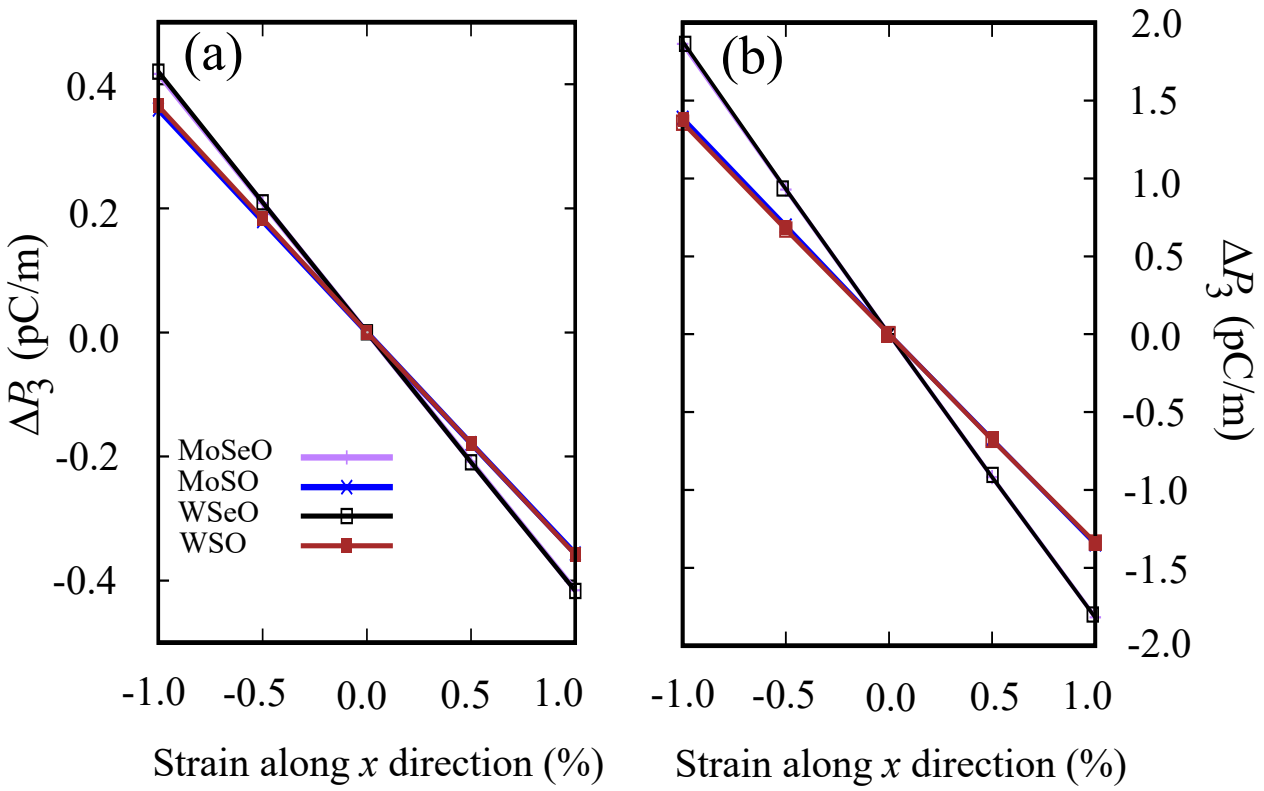

Figure S3: The out-of-plane polarization change (ΔP_3) under the applied uniaxial strain along the x direction of (a) the monolayer and (b) bulk MXO (M = Mo, W; X = S, Se).

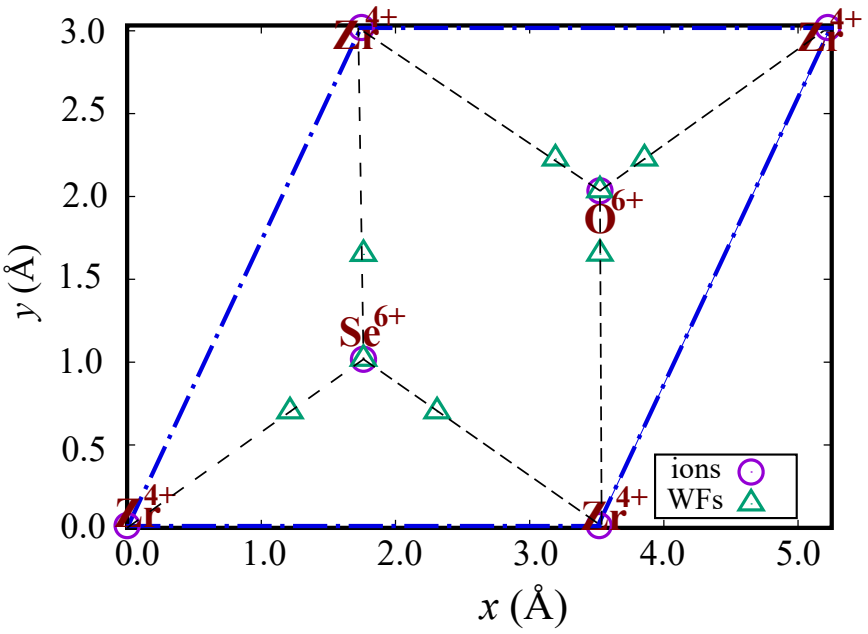

Figure S4: Top view of Wannier function (WF) centers (cyan triangle) of O and Se atoms on ZrSeO.

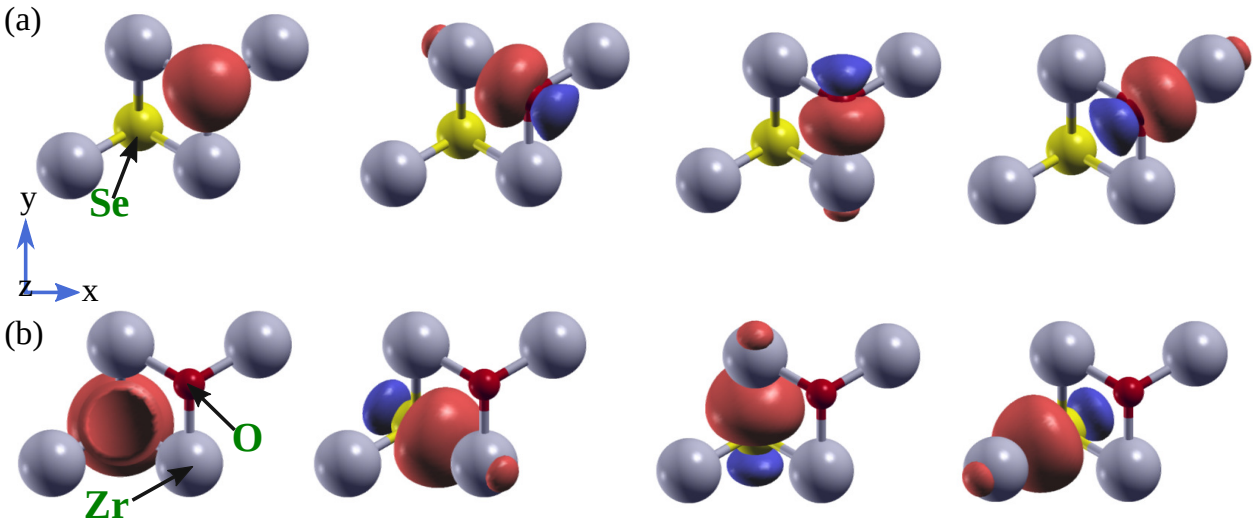

Figure S5: The maximally localized Wannier functions (MLWFs) of (a) O and (b) Se atoms on bulk ZrSeO.