SUPPORTING INFORMATION

Anion Ordering and Relative Impact on the Photocatalytic Activity of $CaTaO_2N$: Insights from First-Principles.

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Table S1: Hole effective mass along each direction. B2 and C have their VBMs on U point.

(Γ = 0.0, 0.0, 0.0; X = 0.5, 0.0, 0.0; Y = 0.0, 0.5, 0.0; Z = 0.0, 0.0, 0.5; S = 0.5, 0.5, 0.0;

T = 0.0, 0.5, 0.5; U = 0.5, 0.0, 0.5; R = 0.5, 0.5, 0.5).

	T→Γ	**T→R**	**T→S**	**T→U**	**T→X**	**T→Y**	**T → Z**	**Ave**
A1	1.74	4.81	0.88	6.11	1.08	1.22	10.55	**1.78**
A2	1.40	4.95	2.53	1.40	1.51	4.64	0.58	**1.51**
B1	3.36	1.79	1.18	2.12	1.38	3.49	2.85	**1.98**
D	0.47	1.25	0.73	0.50	0.37	1.37	0.70	**0.63**
E1	1.62	2.06	-91.0	1.71	10.6	1.57	1.19	**2.15**
E2	7.45	2.94	7.98	1.99	10.95	8.47	1.20	**3.27**
E3	1.30	3.61	3.90	1.30	1.73	4.26	0.57	**1.51**
F1	1.24	1.56	1.85	0.71	0.96	2.01	0.76	**1.12**
F2	4.65	0.85	1.10	0.80	1.69	1.48	0.70	**1.12**
F3	1.25	1.56	1.72	3.17	2.27	2.01	0.76	**1.52**
F4	6.06	1.76	1.73	1.19	3.06	1.60	0.69	**1.54**
	U→Γ	**U→R**	**U→S**	**U→T**	**U→X**	**U→Y**	**U→Z**	**Ave**
B2	7.51	1.21	1.89	2.52	2.54	3.70	5.22	**2.55**
C	1.08	-12.8	2.31	3.16	2.08	1.19	2.36	**2.10**

Table S2: Electron effective mass along each direction.

(BZ special point coordinates as in Table S1)

	Γ→R	**Γ→S**	**Γ→T**	**Γ→U**	**Γ→X**	**Γ→Y**	**Γ→Z**	**Ave**
A1	0.49	0.54	0.55	0.47	0.51	0.64	0.52	**0.53**
A2	0.46	0.58	0.63	0.47	0.68	0.45	0.77	**0.56**
B1	0.39	0.50	0.50	0.41	0.71	0.32	0.69	**0.47**
B2	0.41	0.52	0.51	0.43	0.75	0.33	0.71	**0.48**
C	1.48	0.99	0.71	1.68	0.92	0.71	0.73	**0.93**
D	0.43	0.57	0.53	0.46	0.72	0.40	0.70	**0.52**
E1	0.56	0.57	0.65	0.52	0.53	0.79	0.60	**0.59**
E2	0.82	0.63	1.09	0.73	2.67	0.77	0.82	**0.88**
E3	0.74	0.68	0.75	0.94	0.70	0.68	1.29	**0.79**
F1	0.46	0.63	0.54	0.48	0.84	0.35	0.79	**0.54**
F2	0.56	0.55	0.62	0.54	0.49	0.81	0.60	**0.58**
F3	1.08	0.52	0.54	3.53	0.85	0.35	0.78	**0.68**
F4	0.69	0.59	0.68	0.75	0.63	0.55	0.78	**0.66**

Table S3 Surface energies and bandgaps of each slab model.

	E_{surf} [mJ/m^2]	E_g (slab) [eV]	E_g [eV]
E2(001)_Orich	983.1	1.95	1.84
E2(001)_Nrich	1261.5	1.86	1.84
F2(100)_Orich	1002.6	2.14	2.01
F2(100)_Nrich	1429.1	2.06	2.01
F4(100)_Orich	1077.7	2.15	2.07
F4(100)_Nrich	1337.7	2.15	2.07

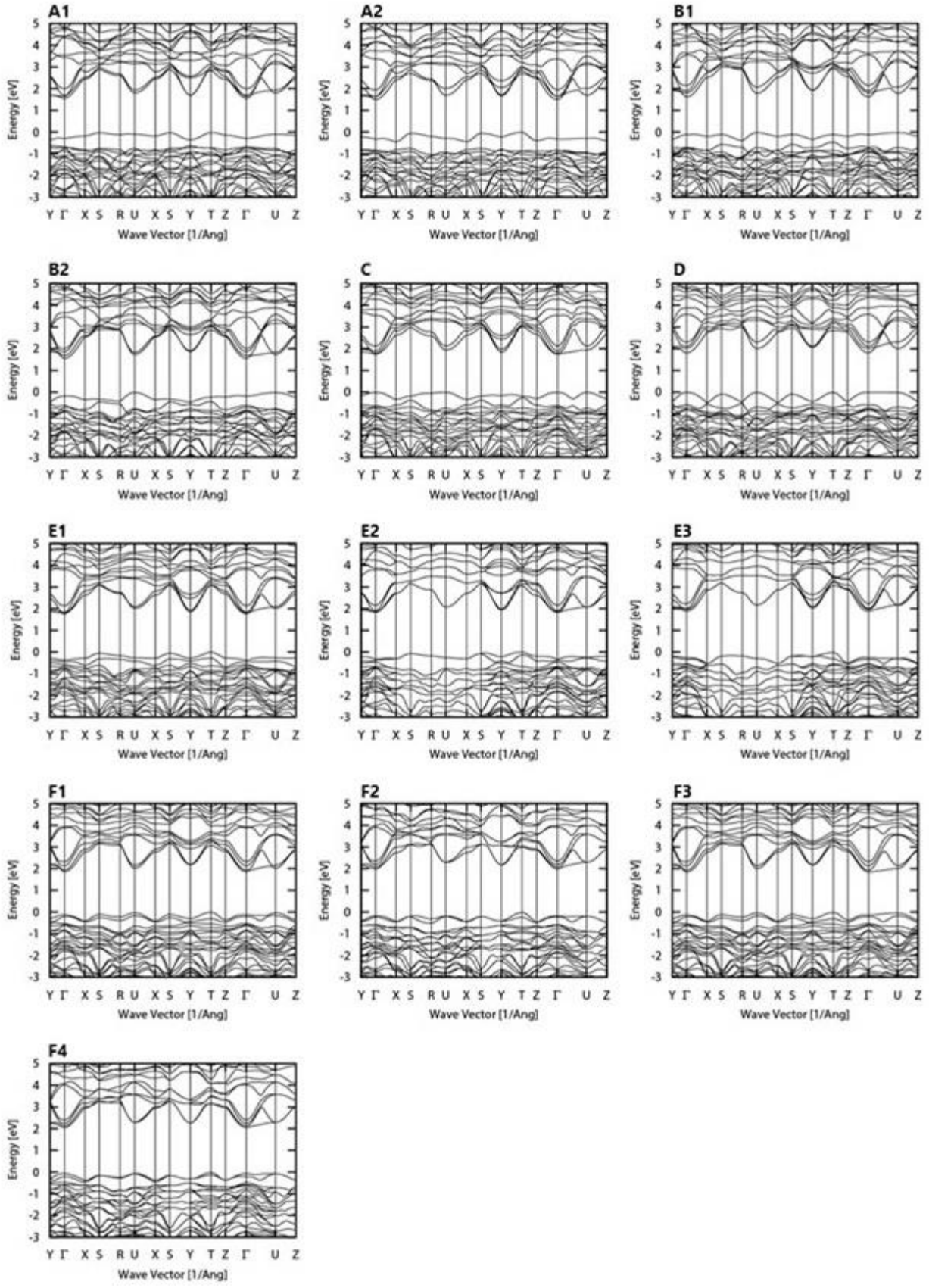

Figure S1 Bandplots of each anion ordering (BZ special point path coordinates as in Table S1).

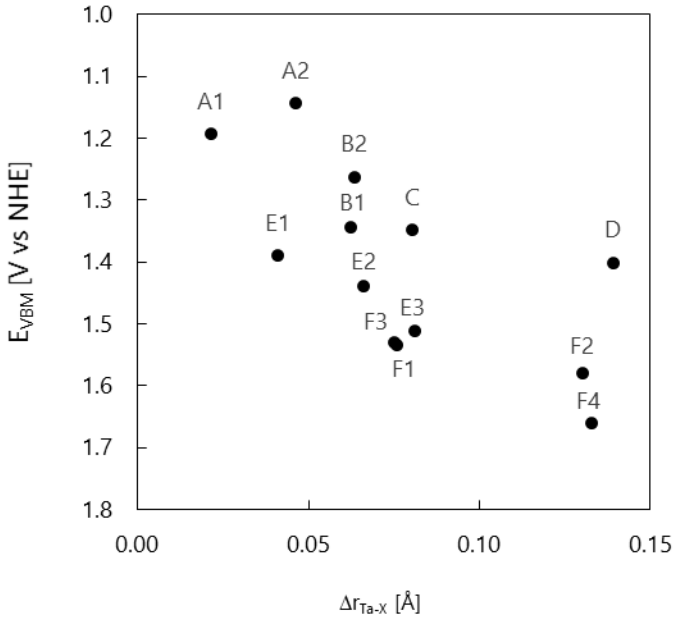

Figure S2. Bond asymmetry and VBM positions of each anion ordering. Δr_{Ta-X} represents the average of the bond difference between two bonds from N or O to Ta (= $(2 \times \Delta r_{Ta-O} + \Delta r_{Ta-N})/3$).