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

Supporting Information

Predicting suitable optoelectronic properties of monoclinic VON semiconductor crystals for photovoltaics using accurate first-principles computations

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Cell parameters of Si, CdTe, and GaAs computed using PBE and compared with available experimental data

Table S1 Computed cell paramters (in Å) for Si, CdTe, and GaAs using PBE. The calculated values are compared to available experimental data.

compound	structure	PBE	Expt.
Si	diamond	5.44	5.43[1]
CdTe	zincblende	6.54	6.46[1]
GaAs	zincblende	5.70	5.65[2]

Atomic positions of the constituting elements in the optimized β- and γ-VON structures

Table S2 Atomic coordinates of V, O, and N elements in the relaxed β-VON structure.

		x	y	z
1	V	1.3739	0.2634	0.8609
2	V	3.3029	4.4408	3.2798
3	V	3.2926	2.6153	0.8188
4	V	1.3842	2.0890	3.3219
5	O	0.3269	1.5087	1.6552
6	O	4.3383	3.8592	0.0235
7	O	4.3499	3.1956	2.4854
8	O	0.3385	0.8451	4.1172
9	N	2.0231	3.5634	2.0118
10	N	2.6428	1.2103	-0.3331
11	N	2.6537	1.1409	2.1288
12	N	2.0340	3.4940	4.4738

Table S3 Atomic coordinates of V, O, and N elements in the relaxed γ-VON structure.

		x	y	z
1	V	3.6879	0	-0.0626
2	V	7.1579	0	-0.7262
3	V	9.5247	1.8186	-1.8805

4	V	1.3211	1.8186	1.0917
5	V	8.0050	0	2.7827
6	V	4.5350	0	3.4462
7	V	2.1682	1.8186	4.6006
8	V	10.3718	1.8186	1.6283
9	O	4.1110	0	1.8036
10	O	1.3932	0	0.8611
11	O	9.9478	1.8186	-0.0143
12	O	7.2300	1.8186	-0.9568
13	O	7.5819	0	0.9165
14	O	10.2998	0	1.8589
15	O	1.7451	1.8186	2.7344
16	O	4.4629	1.8186	3.6768
17	N	5.2595	0	-0.6689
18	N	8.8635	0	-1.7959
19	N	11.0963	1.8186	-2.4868
20	N	3.0267	1.8186	0.0220
21	N	6.4334	0	3.3889
22	N	2.8294	0	4.5159
23	N	0.5966	1.8186	5.2068
24	N	8.6662	1.8186	2.6980

References

(1) O. Madelung, *Semiconductors: Data Handbook,* 3rd ed.; Springer: New York, 2004.

(2) I. Vurgaftman, J. R. Meyer, L. R. Ram-Mohan, *J. Appl. Phys.* **2001**, *89*, 5815–5875.