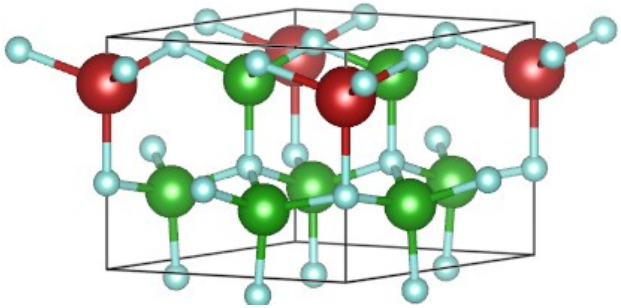
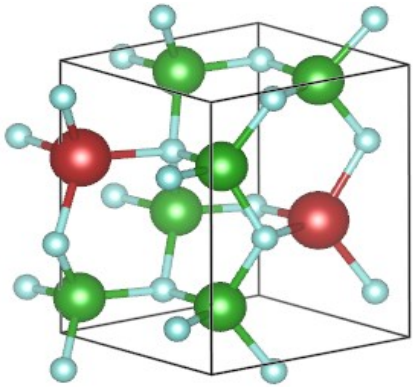
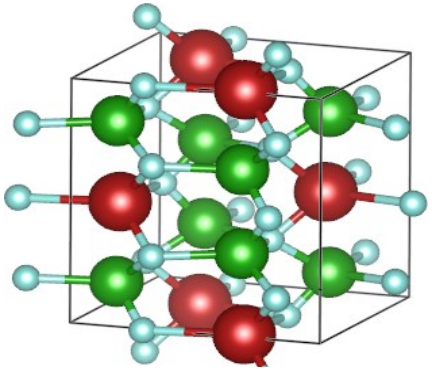
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Structure	Corrected bandgap / eV	Lattice parameter / Å	Wyckoff position
 Al_5InN_6	5.493	$a = 5.451$ $c = 5.054$	Al1 -0.34242 0.00000 0.29396 Al2 0.33333 0.66667 -0.20399 In1 0.00000 0.00000 -0.20021 N1 0.33333 0.66667 0.42142 N2 -0.36820 0.00000 -0.07634 N3 0.00000 0.00000 0.37263
 $Al_6In_2N_8$	4.587	$a = 5.504$ $b = 5.088$ $c = 6.381$ $\beta = 89.88$	Al1 -0.08572 0.01087 0.11993 Al2 0.41300 0.01539 -0.11759 Al3 0.42543 0.01129 0.36901 In1 -0.08929 0.01444 -0.36677 N1 0.09752 0.14455 -0.09969 N2 -0.41071 0.13870 0.12317 N3 -0.45679 0.14170 -0.37324 N4 0.09662 0.09428 0.35356

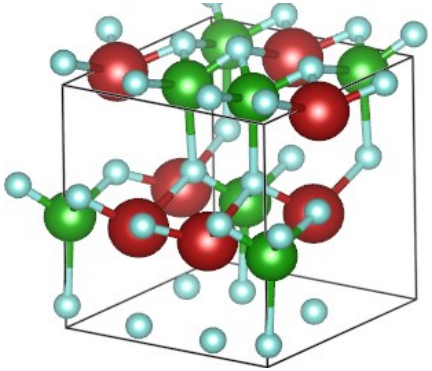


$Al_4In_2N_6$

4.333

$a = 5.568$
$b = 5.551$
$c = 5.146$

Al1	0.32852	0.33649	-0.43980
In1	0.00000	0.32230	-0.44455
N1	0.00000	-0.29973	0.47446
N2	-0.18443	0.14903	0.42509

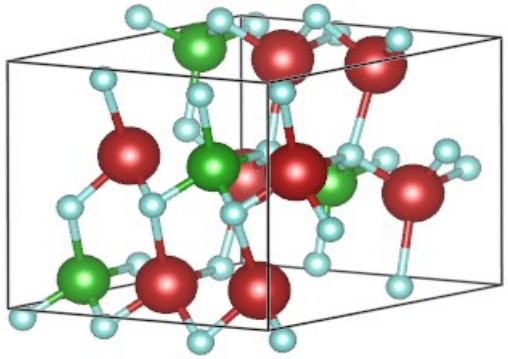
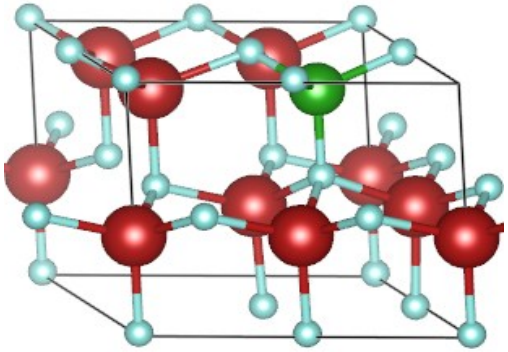


$Al_3In_3N_6$

2.977

$a = 5.698$
$b = 5.268$
$c = 5.680$
$\beta = 90.02$

Al1	-0.38175	0.33766	-0.05310
Al2	-0.03709	0.00000	0.44829
In1	-0.05268	0.32846	0.45018
In2	-0.36844	0.00000	-0.04856
N1	-0.00946	0.00000	0.08889
N2	-0.39523	0.34948	-0.40728
N3	-0.06263	0.31643	0.04231
N4	-0.34955	0.00000	-0.45649

 $Al_2In_4N_6$	1.806	$a = 5.808$ $b = 5.820$ $c = 6.300$ $\beta = 58.48$	Al1 -0.43453 0.42299 0.25064 In1 0.23234 0.40952 0.26002 In2 0.39959 0.08949 -0.26710 N1 0.45835 0.43872 -0.39145 N2 -0.40215 0.11173 0.15781 N3 -0.24435 0.42761 -0.37446
 $AlIn_7N_8$	0.486	$a = 6.889$ $c = 5.539$	Al1 0.33333 0.66667 -0.10470 In1 -0.16731 0.16731 -0.10453 In2 0.49569 -0.49569 0.39568 In3 0.00000 0.00000 0.39473 N1 -0.16799 0.16799 -0.48845 N2 0.48577 -0.48577 0.00704 N3 0.33333 0.66667 -0.44443 N4 0.00000 0.00000 0.01328