Computationally Designed Crystal Structures of the Supertetrahedral Ga_4C and Ga_4Si Solids

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Table S1. Translation vectors in Cartesian coordinates for *cF*-Ga_4C structure.

Vector	*x*	*y*	*z*
$\mathbf{a}_1$	0.0000000000000000	4.1054563532177859	4.1054563532177859
$\mathbf{a}_2$	4.1054563532177859	0.0000000000000000	4.1054563532177859
$\mathbf{a}_3$	4.1054563532177859	4.1054563532177859	0.0000000000000000

Table S2. Direct coordinates of atoms for *cF*-Ga_4C structure.

Atom	η_1	η_2	η_3
Ga_1	0.2237247361844244	0.2237247361844244	0.2237247361844244
Ga_2	0.7824940902812773	0.2237247361844244	0.2237247361844244
Ga_3	0.2237247361844244	0.7824940902812773	0.2237247361844244
Ga_4	0.2237247361844244	0.2237247361844244	0.7824940902812773
C_1	0.3634170747086358	0.3634170747086358	0.3634170747086358

Table S3. Cartesian coordinates of atoms for *cF*-Ga_4C structure.

Atom	*x*	*y*	*z*
Ga_1	3.199711	3.199711	3.199711
Ga_2	5.011202	5.011202	3.199711
Ga_3	5.011202	3.199711	5.011202
Ga_4	3.199711	5.011202	5.011202
C_1	2.052728	2.052728	2.052728

The total energy per primitive unit cell for *cF*-Ga_4C structure is -19.77666039 eV.

Table S4. Translation vectors in Cartesian coordinates for *cF*-Ga_4Si structure.

Vector	*x*	*y*	*z*
$\mathbf{a}_1$	0.0000000000000000	4.5839241451729089	4.5839241451729089
$\mathbf{a}_2$	4.5839241451729089	0.0000000000000000	4.5839241451729089
$\mathbf{a}_3$	4.5839241451729089	4.5839241451729089	0.0000000000000000

Table S5. Direct coordinates of atoms for *cF*-Ga_4Si structure.

Atom	η_1	η_2	η_3
Ga_1	0.8172541926183650	0.2121380354053904	0.2121380354053904
Ga_2	0.2121380354053904	0.8172541926183650	0.2121380354053904
Ga_3	0.2121380354053904	0.2121380354053904	0.8172541926183650
Ga_4	0.2121380354053904	0.2121380354053904	0.2121380354053904
Si_1	0.3634170747086358	0.3634170747086358	0.3634170747086358

Table S6. Cartesian coordinates of atoms for *cF*-Ga_4Si structure.

Atom	*x*	*y*	*z*
Ga_1	3.678874	3.678874	3.678874
Ga_2	5.488975	5.488975	3.678874
Ga_3	5.488975	3.678874	5.488975
Ga_4	3.678874	5.488975	5.488975
Si_1	2.291962	2.291962	2.291962

The total energy per primitive unit cell for *cF*-Ga_4Si structure is -16.31862053 eV.