

SUPPLEMENTARY MATERIALS for
Structure, mechanical and filtration properties of graphyne compounds of the self-intercalated type

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Supplementary materials

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Structural data

Phase designation: 3D-SI- α G1

Space group: $I4/mcm$ (no. 140)

Unit cell parameters: $a = 8.460 \text{ \AA}$, $c = 6.980 \text{ \AA}$

TABLE S1. Nonequivalent atomic positions in unit cell of 3D-SI- α G1 (x , y , z – fractional coordinates)

Atom	Multiplicity	Wyckoff letter	x	y	z
C1	8	h	0.8326	0.3326	0.0000
C2	8	h	0.0509	0.5509	0.0000
C3	16	l	0.2747	0.7747	0.3264

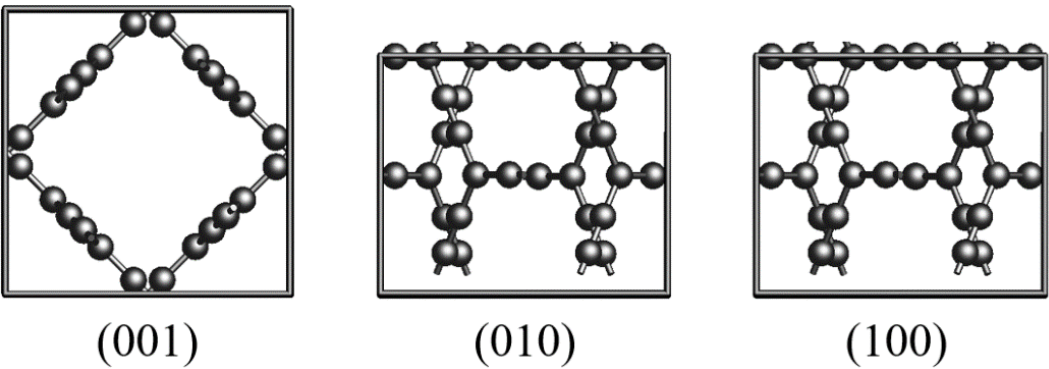


FIG. S1. Projections of crystal structure of 3D-SI- α G1 on general crystallographic planes

Structural data

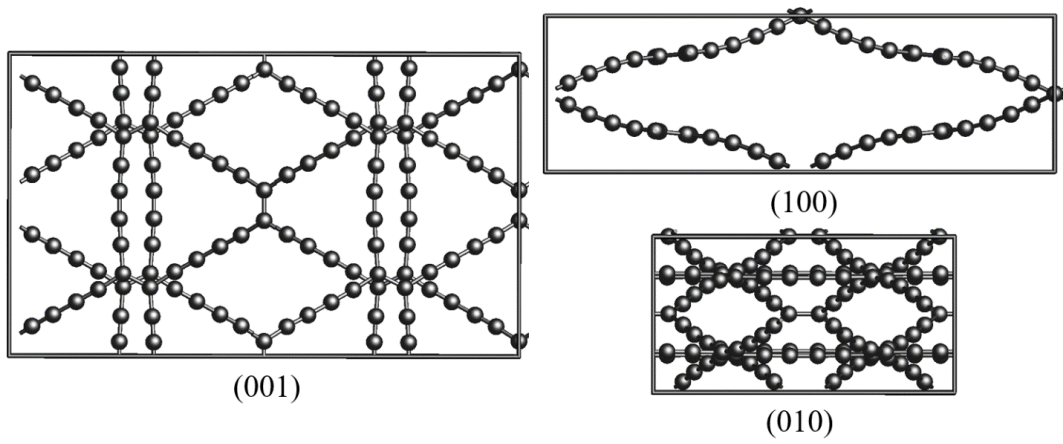
Phase designation: 3D-SI- β 1G2

Space group: $Ibam$ (no. 72)

Unit cell parameters: $a = 14.33 \text{ \AA}$, $b = 24.16 \text{ \AA}$, $c = 7.426 \text{ \AA}$

TABLE S2. Nonequivalent atomic positions in unit cell of 3D-SI- β 1G2 (x, y, z – fractional coordinates)

Atom	Multiplicity	Wyckoff letter	x	y	z
C1	16	k	0.0462	0.7838	0.7633
C2	16	k	0.1314	0.7807	0.7613
C3	16	k	0.2277	0.7766	0.7589
C4	16	k	0.3633	−0.0862	0.8687
C5	16	k	0.4014	−0.0449	−0.0692
C6	16	k	0.2794	0.8248	0.7790
C7	16	k	0.3204	0.8681	0.8139
C8	8	h	0.0503	0.0000	0.0000

FIG. S2. Projections of crystal structure of 3D-SI- β 1G2 on general crystallographic planes