Supporting Information

Two-dimensional fullerene-based monolayer materials assembled by C_{80} and $Sc_3N@C_{80}$

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Supplementary Note1: Calculation of carrier mobility

To characterize the performance of semiconductor transistors, we calculate carrier mobility of 2D monolayers based on the deformation potential theory as follows:

$$\mu = \frac{e\hbar^3 C_{2D}}{k_B T m m_d (E_1)^2} \quad (1)$$

where e is the electron charge, $\hbar$ is the reduced Planck constant, k_B is the Boltzmann constant, T is the temperature, m is the effective mass along the transport direction, $m_d = \sqrt{m_x m_y}$ is the average effective mass, $C_{2D} = 2\left[\partial^2 E / \partial\left(\Delta l / l_0\right)^2\right] / S_0$ is the elastic modulus. E and S_0 stand for the total energy and the area of the xy plane for the unit, respectively. $E_1 = \Delta V / \left(\Delta l / l_0\right)$ represents the deformation potential constant, defined as the shift of band edges induced by strain. ΔV is the energy difference about conduction band minimum (CBM) or valence band maximum (VBM) with the lattice applied by proper dilatation or compression. l_0 and Δl are the lattice constant along the x or y direction and their deformation, respectively.

Supplementary Note2: Calculation of the formation energy and deformation energy by atom-wise energies

The formation energy ($E_{\text{f - atom}}$) and deformation energy ($E_{\text{d - atom}}$) are defined by atom-wise energies, as follows:

$$E_{\text{f - atom}} = E_{2D}/n' - E_{\text{C}} \tag{2}$$

where E_{2D} and E_{C} are the energies of 2D monolayer and C atoms, respectively. n' is the number of C atoms in the unit cell.

$$E_{\text{d - atom}} = E_{\text{2D - def - cage}}/n' - E_{\text{cage}}/n' \tag{3}$$

where $E_{\text{2D - def - cage}}$ and E_{cage} are the energies of the deformed cage in 2D structures and the standalone cage in its ground state configuration, respectively. n' is the number of C atoms in the unit cell.

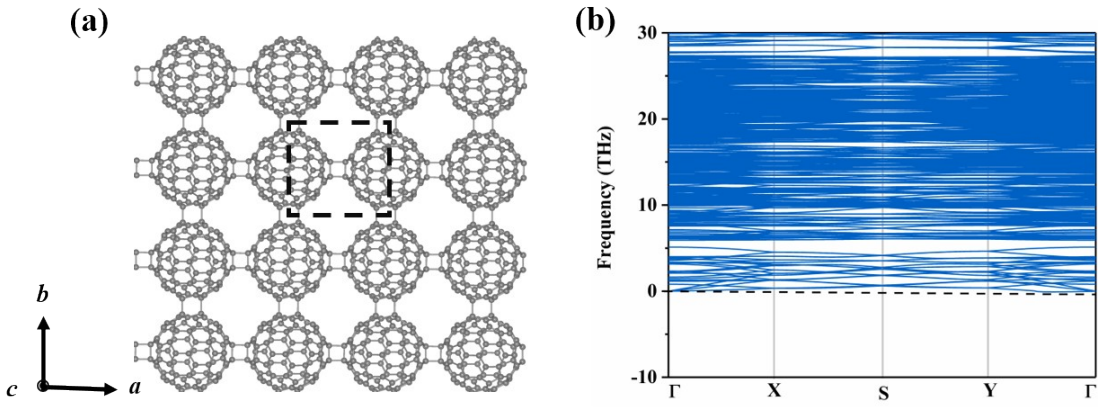

Fig. S1 Crystal structure and phonon spectra of monolayer of γ-C_{80}-2D.

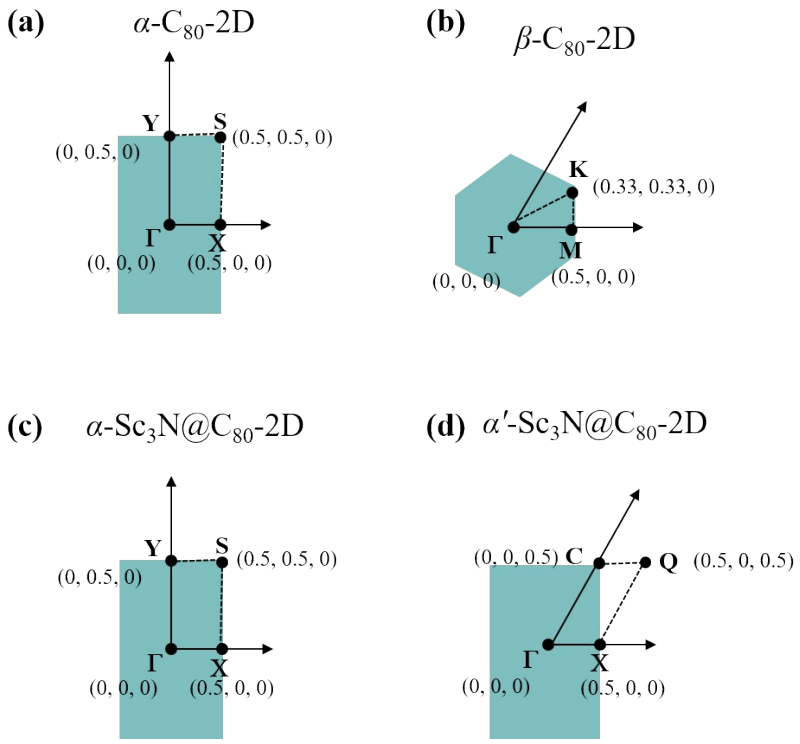

Fig. S2 2D rectangular Brillouin zones of (a) α-C_{80}-2D, (b) β-C_{80}-2D, (c) α-$Sc_3N@C_{80}$-2D and (d)α'-$Sc_3N@C_{80}$-2D crystal lattices.

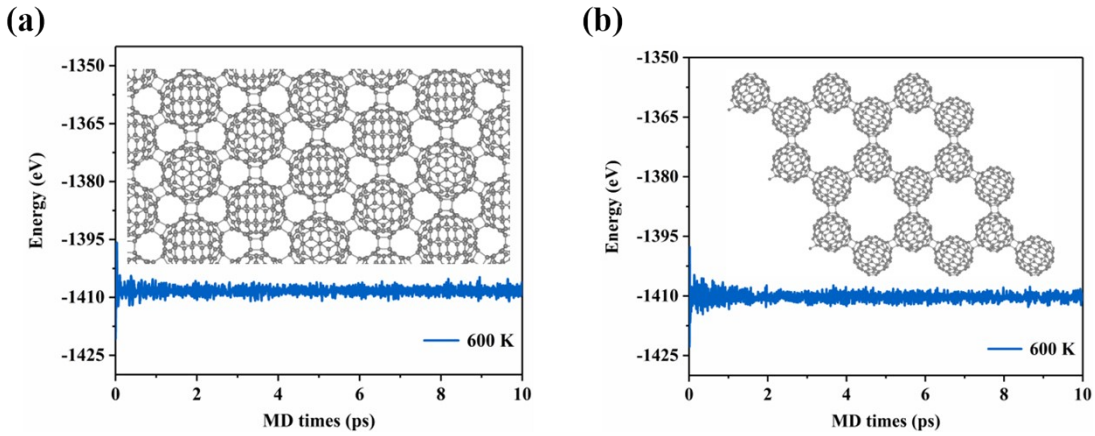

Fig. S3 Energy profile during AIMD simulation at 600 K for (a) α-C_{80}-2D and (b) β-C_{80}-2D.

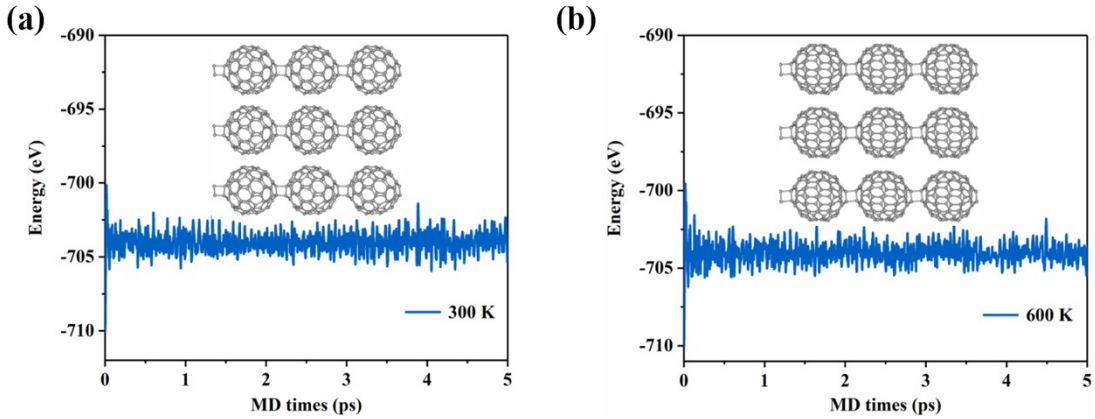

Fig. S4 Energy profiles and snapshot structures at 5 ps for γ-C_{80}-2D at (a) 300 K, (b) 600 K.

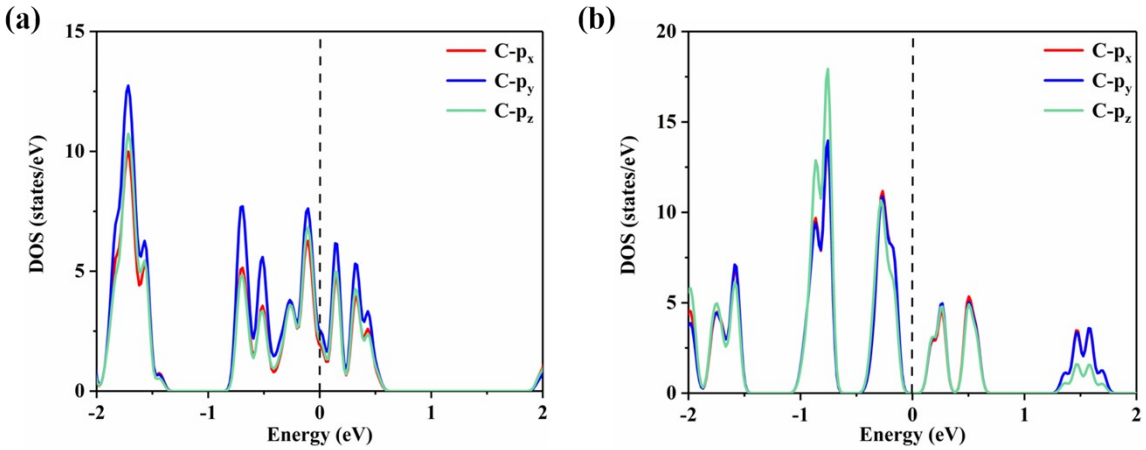

Fig. S5 The *p*-orbital-resolved density of states for C atoms in (a) *α*-C_{80}-2D and (b) *β*-C_{80}-2D.

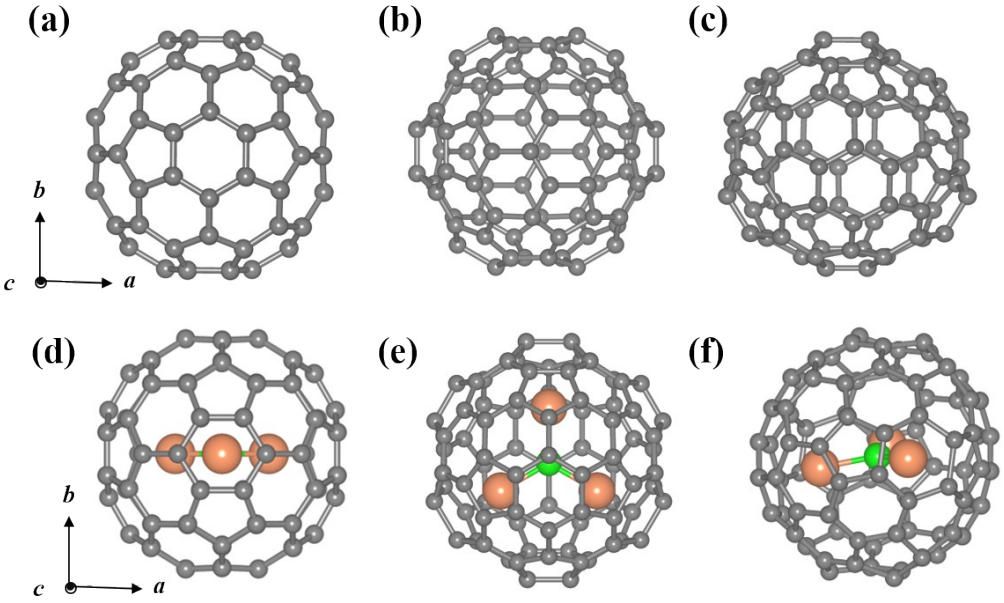

Fig. S6 Freestanding cages of (a) C_{80} and (d) $Sc_3N@C_{80}$. Deformed C_{80} or $Sc_3N@C_{80}$ cages directly taken from 2D monolayer structures of (b) α-C_{80}, (c) β-C_{80}, (e) α-$Sc_3N@C_{80}$ and (f) α'-$Sc_3N@C_{80}$.

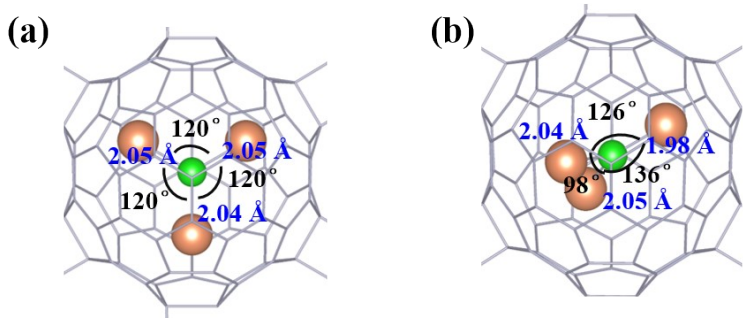

Fig. S7 The Sc−N bond lengths (blue) and Sc−N−Sc angles (black) of (a) α-$Sc_3N@C_{80}$-2D and (b) α'-$Sc_3N@C_{80}$-2D.

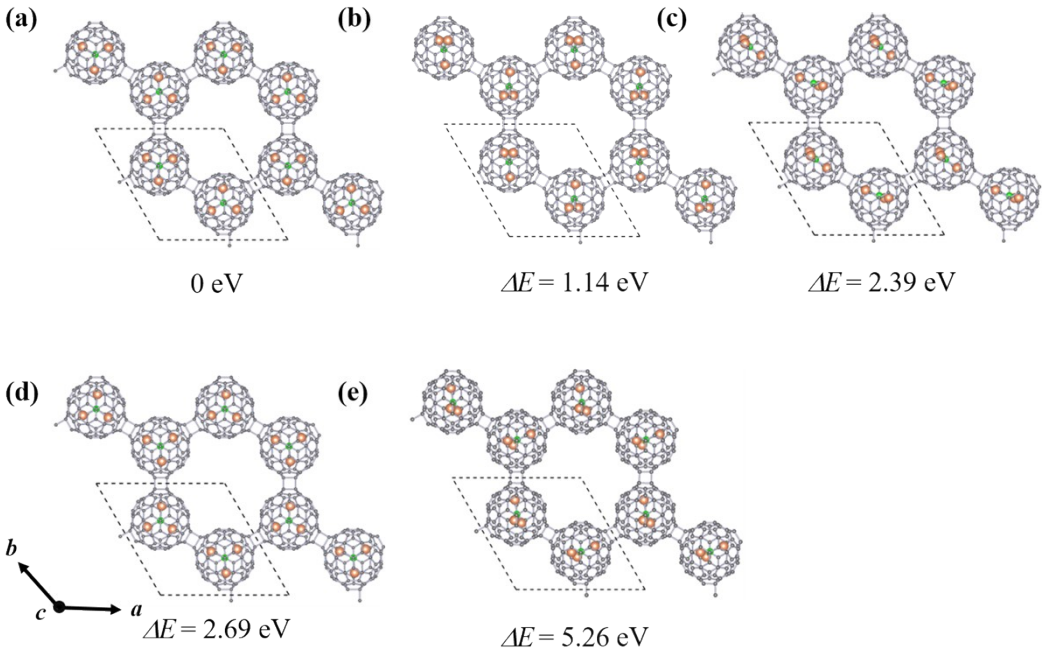

Fig. S8 Typical low-lying isomers of β-$Sc_3N@C_{80}$-2D monolayers.

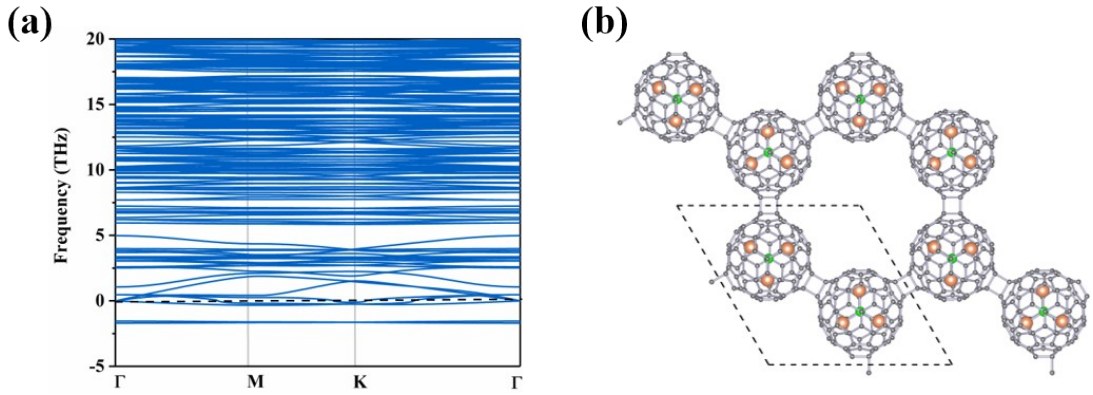

Fig. S9 Crystal structure and phonon spectra of the lowest energy β-$Sc_3N@C_{80}$-2D monolayer.

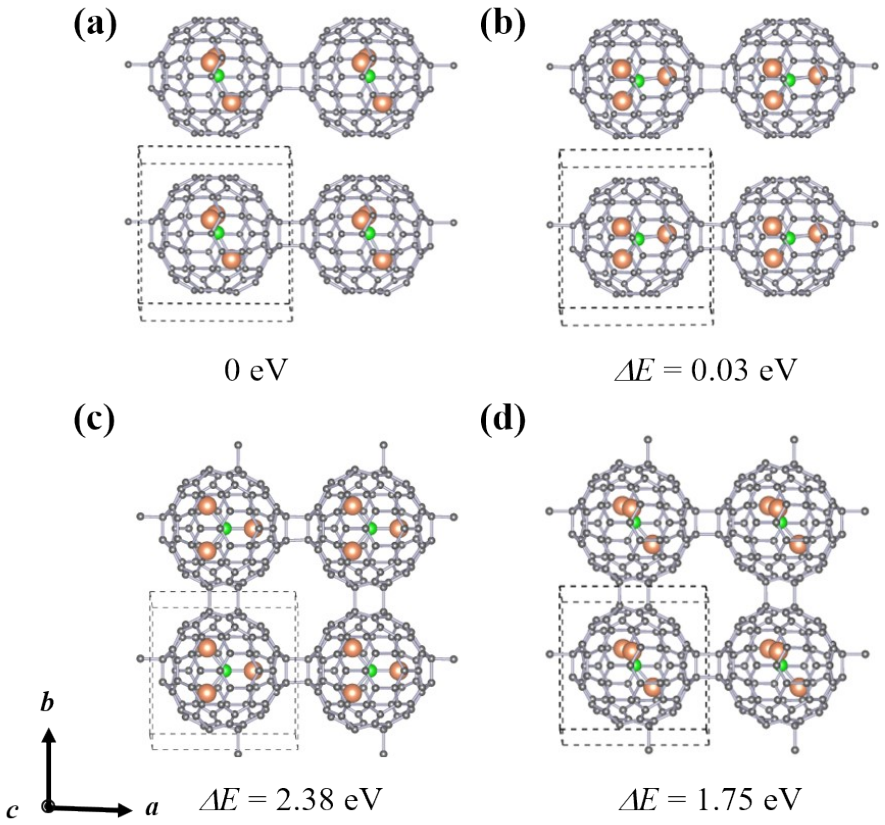

Fig. S10 Typical low-lying isomers of γ-$Sc_3N@C_{80}$-2D monolayers.

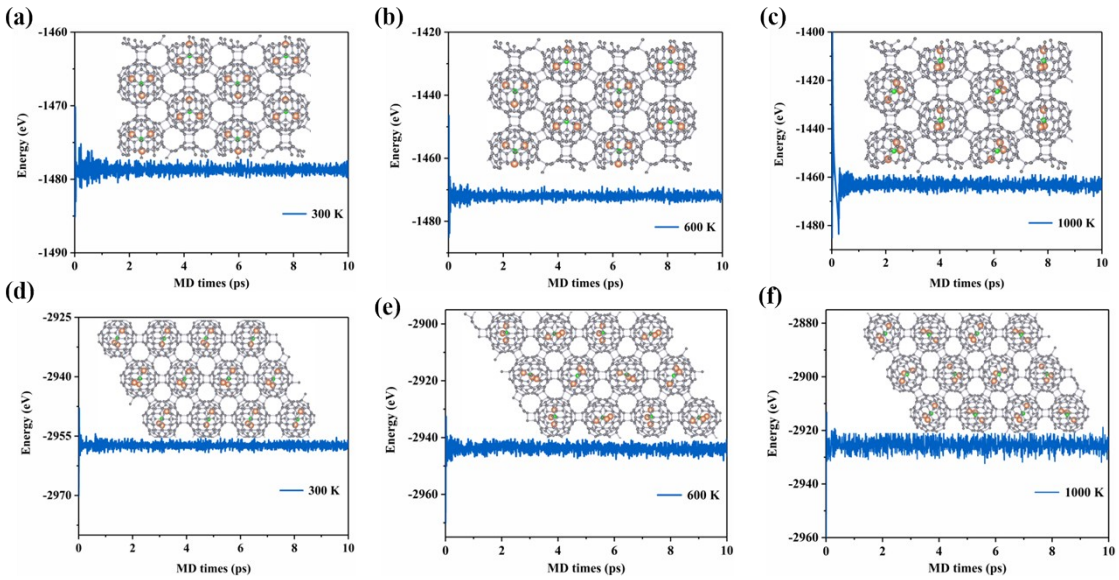

Fig. S11 Energy profiles and snapshot structures at 10 ps for α-$Sc_3N@C_{80}$-2D system at (a) 300 K, (b) 600 K, and (c) 1000 K and for α'-$Sc_3N@C_{80}$-2D system at (d) 300 K, (e) 600 K, and (f) 1000 K.

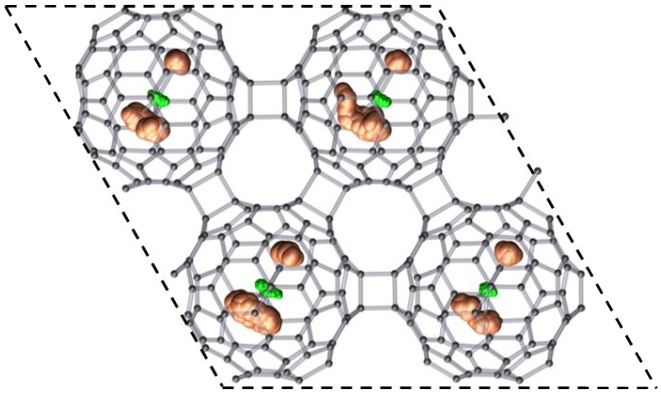

Fig. S12 Schematic representation of disorder states for α'-$Sc_3N@C_{80}$-2D crystal at 300K. The representative rotational operation of the Sc_3N species for α'-$Sc_3N@C_{80}$-2D phase are available in the movies.

Table S1. The Sc−N bond lengths (R_{Sc-N}) of Sc_3N clusters and electronic energy-gap by using the PBE (E_g) for α-$Sc_3N@C_{80}$-2D material under different U_{eff} (Sc) correction.

U_{eff} (Sc)	0	1	2	3	4
R_{Sc-N} (Å)	2.05	2.05	2.05	2.05	2.05
E_g (eV)	0.08	0.13	0.13	0.13	0.13

Table S2. The deformation energy ($E_{\text{d-atom}}$), and formation energy ($E_{\text{f-atom}}$) defined with atom-wise energies of 2D monolayers.

Monolayer	$E_{\text{d-atom}}$ (eV/atom)	$E_{\text{f-atom}}$ (eV/atom)
qTP-C_{60}	0.08	–6.95
qHP-C_{60}	0.09	–6.95
α-C_{80}-2D	0.09	–7.01
β-C_{80}-2D	0.04	–6.99
γ-C_{80}-2D	0.07	–6.98

Table S3. Effective mass (m), deformation potential constant (E_1), elastic modulus (C), carrier mobility (μ) for β-C_{80}-2D, α-$Sc_3N@C_{80}$-2D and α'-$Sc_3N@C_{80}$-2D monolayers.

Monolayer	Direction	Carrier	m (m_0)	E_1 (eV)	C (J m^{-2})	μ (10^3 cm^2 V^{-1} s^{-1})
β-C_{80}-2D	x	hole	0.42	2.66	91.54	1.60
		electron	0.83	1.33		1.84
	y	hole	0.39	1.61	65.76	3.37
		electron	0.62	0.78		5.57
α-$Sc_3N@C_{80}$-2D	x	hole	1.33	3.07	190.50	0.25
		electron	0.85	4.85		0.25
	y	hole	1.28	6.06	197.39	0.07
		electron	0.75	4.75		0.31
α'-$Sc_3N@C_{80}$-2D	x	hole	1.10	6.01	187.70	0.11
		electron	1.36	3.73		0.17
	y	hole	0.80	8.92	191.20	0.07
		electron	1.10	5.68		0.09

DFT optimized coordinates (Å) and lattice parameters of 2D monolayers

α-C_{80}-2D monolayer with a = 17.76 Å, b = 10.25 Å, c = 34.97 Å, α = 90°, β = 90°, γ = 90°

	x	y	z
C	0.2663	0.6435	0.4898
C	0.7337	0.3565	0.5102
C	0.2337	0.1435	0.5102
C	0.7663	0.8565	0.4898
C	0.2337	0.8565	0.4898
C	0.7663	0.1435	0.5102
C	0.2663	0.3565	0.5102
C	0.7337	0.6435	0.4898
C	0.7155	0.5901	0.5294
C	0.2845	0.4099	0.4706
C	0.7845	0.0901	0.4706
C	0.2155	0.9099	0.5294
C	0.7845	0.9099	0.5294
C	0.2155	0.0901	0.4706
C	0.7155	0.4099	0.4706
C	0.2845	0.5901	0.5294
C	0.3284	0.6817	0.5499
C	0.6716	0.3183	0.4501
C	0.1716	0.1817	0.4501
C	0.8284	0.8183	0.5499
C	0.1716	0.8183	0.5499
C	0.8284	0.1817	0.4501
C	0.3284	0.3183	0.4501
C	0.6716	0.6817	0.5499
C	0.6888	0.7788	0.4881
C	0.3112	0.2212	0.5119
C	0.8112	0.2788	0.5119
C	0.1888	0.7212	0.4881
C	0.8112	0.7212	0.4881
C	0.1888	0.2788	0.5119
C	0.6888	0.2212	0.5119
C	0.3112	0.7788	0.4881
C	0.3674	0.7931	0.4561
C	0.6326	0.2069	0.5439
C	0.1326	0.2931	0.5439
C	0.8674	0.7069	0.4561
C	0.1326	0.7069	0.4561
C	0.8674	0.2931	0.5439
C	0.3674	0.2069	0.5439

C	0.6326	0.7931	0.4561
C	0.6301	0.6465	0.5831
C	0.3699	0.3535	0.4169
C	0.8699	0.1465	0.4169
C	0.1301	0.8535	0.5831
C	0.8699	0.8535	0.5831
C	0.1301	0.1465	0.4169
C	0.6301	0.3535	0.4169
C	0.3699	0.6465	0.5831
C	0.3672	0.7023	0.4257
C	0.6328	0.2977	0.5743
C	0.1328	0.2023	0.5743
C	0.8672	0.7977	0.4257
C	0.1328	0.7977	0.4257
C	0.8672	0.2023	0.5743
C	0.3672	0.2977	0.5743
C	0.6328	0.7023	0.4257
C	0.6330	0.5142	0.5945
C	0.3670	0.4858	0.4055
C	0.8670	0.0142	0.4055
C	0.1330	0.9858	0.5945
C	0.8670	0.9858	0.5945
C	0.1330	0.0142	0.4055
C	0.6330	0.4858	0.4055
C	0.3670	0.5142	0.5945
C	0.4352	0.7197	0.5910
C	0.5648	0.2803	0.4090
C	0.0648	0.2197	0.4090
C	0.9352	0.7803	0.5910
C	0.0648	0.7803	0.5910
C	0.9352	0.2197	0.4090
C	0.4352	0.2803	0.4090
C	0.5648	0.7197	0.5910
C	0.5656	0.8601	0.4627
C	0.4344	0.1399	0.5373
C	0.9344	0.3601	0.5373
C	0.0656	0.6399	0.4627
C	0.9344	0.6399	0.4627
C	0.0656	0.3601	0.5373
C	0.5656	0.1399	0.5373
C	0.4344	0.8601	0.4627
C	0.4594	0.8193	0.5652
C	0.5406	0.1807	0.4348
C	0.0406	0.3193	0.4348

C	0.9594	0.6807	0.5652
C	0.0406	0.6807	0.5652
C	0.9594	0.3193	0.4348
C	0.4594	0.1807	0.4348
C	0.5406	0.8193	0.5652
C	0.5445	0.9224	0.5000
C	0.4555	0.0776	0.5000
C	0.9555	0.4224	0.5000
C	0.0445	0.5776	0.5000
C	0.9555	0.5776	0.5000
C	0.0445	0.4224	0.5000
C	0.5445	0.0776	0.5000
C	0.4555	0.9224	0.5000
C	0.4317	0.6815	0.4022
C	0.5683	0.3185	0.5978
C	0.0683	0.1815	0.5978
C	0.9317	0.8185	0.4022
C	0.0683	0.8185	0.4022
C	0.9317	0.1815	0.5978
C	0.4317	0.3185	0.5978
C	0.5683	0.6815	0.4022
C	0.5682	0.4519	0.6104
C	0.4318	0.5481	0.3896
C	0.9318	0.9519	0.3896
C	0.0682	0.0481	0.6104
C	0.9318	0.0481	0.6104
C	0.0682	0.9519	0.3896
C	0.5682	0.5481	0.3896
C	0.4318	0.4519	0.6104
C	0.2854	0.5423	0.4604
C	0.7146	0.4577	0.5396
C	0.2146	0.0423	0.5396
C	0.7854	0.9577	0.4604
C	0.2146	0.9577	0.4604
C	0.7854	0.0423	0.5396
C	0.2854	0.4577	0.5396
C	0.7146	0.5423	0.4604
C	0.3268	0.5792	0.4278
C	0.6732	0.4208	0.5722
C	0.1732	0.0792	0.5722
C	0.8268	0.9208	0.4278
C	0.1732	0.9208	0.4278
C	0.8268	0.0792	0.5722
C	0.3268	0.4208	0.5722

C	0.6732	0.5792	0.4278
C	0.3512	0.7861	0.5260
C	0.6488	0.2139	0.4740
C	0.1488	0.2861	0.4740
C	0.8512	0.7139	0.5260
C	0.1488	0.7139	0.5260
C	0.8512	0.2861	0.4740
C	0.3512	0.2139	0.4740
C	0.6488	0.7861	0.5260
C	0.4179	0.8530	0.5325
C	0.5821	0.1470	0.4675
C	0.0821	0.3530	0.4675
C	0.9179	0.6470	0.5325
C	0.0821	0.6470	0.5325
C	0.9179	0.3530	0.4675
C	0.4179	0.1470	0.4675
C	0.5821	0.8530	0.5325
C	0.5000	0.8356	0.4410
C	0.5000	0.1644	0.5590
C	0.0000	0.3356	0.5590
C	0.0000	0.6644	0.4410
C	0.5000	0.6575	0.6069
C	0.5000	0.3425	0.3931
C	0.0000	0.1575	0.3931
C	0.0000	0.8425	0.6069
C	0.5000	0.7458	0.4100
C	0.5000	0.2542	0.5900
C	0.0000	0.2458	0.5900
C	0.0000	0.7542	0.4100
C	0.5000	0.5215	0.6157
C	0.5000	0.4785	0.3843
C	0.0000	0.0215	0.3843
C	0.0000	0.9785	0.6157

β-C_{80}-2D network with a =17.52 Å, b = 17.52 Å, c = 35.00 Å, α = 90°, β = 90°, γ = 120°

	x	y	z
C	0.3992	0.1592	0.4872
C	0.6008	0.8408	0.5128
C	0.8408	0.2400	0.4872
C	0.1592	0.7600	0.5128
C	0.7600	0.6008	0.4872
C	0.2400	0.3992	0.5128

C	0.1592	0.3992	0.5128
C	0.8408	0.6008	0.4872
C	0.2400	0.8408	0.5128
C	0.7600	0.1592	0.4872
C	0.6008	0.7600	0.5128
C	0.3992	0.2400	0.4872
C	0.4185	0.1431	0.5256
C	0.5815	0.8569	0.4744
C	0.8569	0.2755	0.5256
C	0.1431	0.7245	0.4744
C	0.7245	0.5815	0.5256
C	0.2755	0.4185	0.4744
C	0.1431	0.4185	0.4744
C	0.8569	0.5815	0.5256
C	0.2755	0.8569	0.4744
C	0.7245	0.1431	0.5256
C	0.5815	0.7245	0.4744
C	0.4185	0.2755	0.5256
C	0.4335	0.2990	0.4555
C	0.5665	0.7010	0.5445
C	0.7010	0.1345	0.4555
C	0.2990	0.8655	0.5445
C	0.8655	0.5665	0.4555
C	0.1345	0.4335	0.5445
C	0.2990	0.4335	0.5445
C	0.7010	0.5665	0.4555
C	0.1345	0.7010	0.5445
C	0.8655	0.2990	0.4555
C	0.5665	0.8655	0.5445
C	0.4335	0.1345	0.4555
C	0.4598	0.2707	0.4224
C	0.5402	0.7293	0.5776
C	0.7293	0.1891	0.4224
C	0.2707	0.8109	0.5776
C	0.8109	0.5402	0.4224
C	0.1891	0.4598	0.5776
C	0.2707	0.4598	0.5776
C	0.7293	0.5402	0.4224
C	0.1891	0.7293	0.5776
C	0.8109	0.2707	0.4224
C	0.5402	0.8109	0.5776
C	0.4598	0.1891	0.4224
C	0.5321	0.3355	0.5891
C	0.4679	0.6645	0.4109

C	0.6645	0.1966	0.5891
C	0.3355	0.8035	0.4109
C	0.8034	0.4679	0.5891
C	0.1966	0.5321	0.4109
C	0.3355	0.5321	0.4109
C	0.6645	0.4679	0.5891
C	0.1966	0.6645	0.4109
C	0.8034	0.3355	0.5891
C	0.4679	0.8035	0.4109
C	0.5321	0.1966	0.5891
C	0.3906	0.4770	0.5371
C	0.6094	0.5230	0.4629
C	0.5230	0.9136	0.5371
C	0.4770	0.0864	0.4629
C	0.0864	0.6094	0.5371
C	0.9136	0.3906	0.4629
C	0.4770	0.3906	0.4629
C	0.5230	0.6094	0.5371
C	0.9136	0.5230	0.4629
C	0.0864	0.4770	0.5371
C	0.6094	0.0864	0.4629
C	0.3906	0.9136	0.5371
C	0.5212	0.3958	0.5651
C	0.4788	0.6042	0.4349
C	0.6042	0.1253	0.5651
C	0.3958	0.8747	0.4349
C	0.8747	0.4788	0.5651
C	0.1253	0.5212	0.4349
C	0.3958	0.5212	0.4349
C	0.6042	0.4788	0.5651
C	0.1253	0.6042	0.4349
C	0.8747	0.3958	0.5651
C	0.4788	0.8747	0.4349
C	0.5212	0.1253	0.5651
C	0.4301	0.4794	0.5003
C	0.5699	0.5206	0.4997
C	0.5206	0.9507	0.5003
C	0.4794	0.0493	0.4997
C	0.0493	0.5699	0.5003
C	0.9507	0.4301	0.4997
C	0.4794	0.4301	0.4997
C	0.5206	0.5699	0.5003
C	0.9507	0.5206	0.4997
C	0.0493	0.4794	0.5003

C	0.5699	0.0493	0.4997
C	0.4301	0.9507	0.5003
C	0.4655	0.3664	0.5331
C	0.5345	0.6336	0.4669
C	0.6336	0.0990	0.5331
C	0.3664	0.9010	0.4669
C	0.9010	0.5345	0.5331
C	0.0990	0.4655	0.4669
C	0.3664	0.4655	0.4669
C	0.6336	0.5345	0.5331
C	0.0990	0.6336	0.4669
C	0.9010	0.3664	0.5331
C	0.5345	0.9010	0.4669
C	0.4655	0.0990	0.5331
C	0.5301	0.3313	0.3984
C	0.4699	0.6687	0.6016
C	0.6687	0.1988	0.3984
C	0.3313	0.8012	0.6016
C	0.8012	0.4699	0.3984
C	0.1988	0.5301	0.6016
C	0.3313	0.5301	0.6016
C	0.6687	0.4699	0.3984
C	0.1988	0.6687	0.6016
C	0.8012	0.3313	0.3984
C	0.4699	0.8012	0.6016
C	0.5301	0.1988	0.3984
C	0.4297	0.2148	0.5490
C	0.5703	0.7852	0.4510
C	0.7852	0.2149	0.5490
C	0.2148	0.7851	0.4510
C	0.7851	0.5703	0.5490
C	0.2149	0.4297	0.4510
C	0.4883	0.2442	0.5806
C	0.5117	0.7558	0.4194
C	0.7558	0.2441	0.5806
C	0.2442	0.7559	0.4194
C	0.7559	0.5117	0.5806
C	0.2441	0.4883	0.4194
C	0.5740	0.2870	0.3835
C	0.4260	0.7130	0.6165
C	0.7130	0.2870	0.3835
C	0.2870	0.7130	0.6165
C	0.7130	0.4260	0.3835
C	0.2870	0.5740	0.6165

C	0.5499	0.0999	0.4406
C	0.4501	0.9001	0.5594
C	0.9001	0.4501	0.4406
C	0.0999	0.5499	0.5594
C	0.5500	0.4501	0.4406
C	0.4501	0.5499	0.5594
C	0.5783	0.1565	0.4075
C	0.4217	0.8435	0.5925
C	0.8435	0.4217	0.4075
C	0.1565	0.5783	0.5925
C	0.5783	0.4217	0.4075
C	0.4217	0.5783	0.5925
C	0.6204	0.2407	0.6036
C	0.3796	0.7593	0.3964
C	0.7593	0.3796	0.6036
C	0.2407	0.6204	0.3964
C	0.6204	0.3796	0.6036
C	0.3796	0.6204	0.3964
C	0.3333	0.6667	0.6228
C	0.6667	0.3333	0.3772
C	0.3333	0.6667	0.3899
C	0.6667	0.3333	0.6101

γ-C_{80}-2D network with a =10.19 Å, b = 9.90 Å, c = 34.97 Å, α = 87.85°, β = 90.37°, γ = 90.06°

C	0.3061	0.1692	0.5642
C	0.5198	0.7536	0.3841
C	0.4018	0.0816	0.5379
C	0.4582	0.6391	0.3660
C	0.2130	0.7395	0.4474
C	0.1738	0.4168	0.5790
C	0.1387	0.6216	0.4546
C	0.7528	0.8100	0.5134
C	0.3011	0.2737	0.4094
C	0.6335	0.8774	0.5113
C	0.3218	0.3909	0.3812
C	0.6543	0.2705	0.3978
C	0.9217	0.5804	0.5001
C	0.7251	0.3939	0.3902
C	0.6932	0.1838	0.4356
C	0.4807	0.7275	0.6160
C	0.5975	0.0902	0.4619
C	0.5421	0.6090	0.6341

C	0.7875	0.7280	0.5528
C	0.8260	0.4348	0.4209
C	0.8615	0.6117	0.5454
C	0.2479	0.8126	0.4868
C	0.6984	0.2536	0.5905
C	0.3674	0.8793	0.4889
C	0.6779	0.3643	0.6187
C	0.3452	0.2474	0.6021
C	0.0786	0.5802	0.5000
C	0.2748	0.3690	0.6097
C	0.4234	0.8184	0.4124
C	0.4578	0.1313	0.4525
C	0.4228	0.2012	0.4122
C	0.4586	0.8788	0.4527
C	0.2117	0.2245	0.5330
C	0.1432	0.3464	0.5399
C	0.7878	0.2322	0.4668
C	0.8565	0.3556	0.4600
C	0.5281	0.5157	0.3600
C	0.6627	0.5145	0.3714
C	0.2559	0.5122	0.3906
C	0.1622	0.5080	0.4278
C	0.6939	0.8308	0.4358
C	0.4802	0.2464	0.6159
C	0.5982	0.9184	0.4621
C	0.5418	0.3609	0.6340
C	0.7870	0.2605	0.5526
C	0.8262	0.5832	0.4210
C	0.8613	0.3784	0.5454
C	0.2472	0.1900	0.4866
C	0.6989	0.7263	0.5906
C	0.3665	0.1226	0.4887
C	0.6782	0.6091	0.6188
C	0.3457	0.7295	0.6022
C	0.0783	0.4196	0.4999
C	0.2749	0.6061	0.6098
C	0.3068	0.8162	0.5644
C	0.5193	0.2725	0.3840
C	0.4025	0.9098	0.5381
C	0.4579	0.3910	0.3659
C	0.2125	0.2720	0.4472
C	0.1740	0.5652	0.5791
C	0.1385	0.3883	0.4546
C	0.7521	0.1874	0.5132

C	0.3016	0.7464	0.4095
C	0.6326	0.1207	0.5111
C	0.3221	0.6356	0.3812
C	0.6548	0.7526	0.3979
C	0.9215	0.4198	0.5000
C	0.7252	0.6310	0.3902
C	0.5766	0.1817	0.5876
C	0.5423	0.8687	0.5475
C	0.5772	0.7988	0.5878
C	0.5414	0.1212	0.5473
C	0.7883	0.7755	0.4670
C	0.8568	0.6536	0.4601
C	0.2122	0.7678	0.5332
C	0.1435	0.6444	0.5400
C	0.4719	0.4843	0.6400
C	0.3373	0.4855	0.6286
C	0.7441	0.4878	0.6094
C	0.8378	0.4920	0.5722

α-$Sc_3N@C_{80}$-2D network with a =17.88 Å, b = 10.31 Å, c = 34.97 Å, α = 90°, β = 90°, γ = 90°

	x	y	z
C	0.0150	0.3914	0.5096
C	0.4649	0.3370	0.4707
C	0.0790	0.4286	0.4499
C	0.4383	0.5283	0.5113
C	0.1169	0.5435	0.5434
C	0.3798	0.3935	0.4166
C	0.1164	0.4494	0.5737
C	0.3827	0.2617	0.4054
C	0.1856	0.4665	0.4087
C	0.3152	0.6081	0.5367
C	0.2098	0.5690	0.4336
C	0.2941	0.6691	0.4993
C	0.1823	0.4281	0.5969
C	0.3183	0.2001	0.3894
C	0.0326	0.2906	0.5390
C	0.0762	0.3288	0.5717
C	0.1028	0.5321	0.4740
C	0.1693	0.5997	0.4670
C	0.9836	0.8947	0.4894
C	0.5349	0.8412	0.5285
C	0.9228	0.9333	0.5495

C	0.5610	0.0281	0.4878
C	0.8832	0.0420	0.4560
C	0.6196	0.8974	0.5828
C	0.8840	0.9532	0.4253
C	0.6177	0.7658	0.5936
C	0.8146	0.9688	0.5902
C	0.6838	0.1103	0.4629
C	0.7901	0.0713	0.5649
C	0.7036	0.1774	0.4997
C	0.8184	0.9313	0.4024
C	0.6821	0.7038	0.6095
C	0.9644	0.7948	0.4602
C	0.9243	0.8317	0.4273
C	0.8988	0.0353	0.5253
C	0.8341	0.1083	0.5323
C	0.9850	0.6087	0.5096
C	0.5351	0.6630	0.4707
C	0.9209	0.5715	0.4499
C	0.5617	0.4716	0.5113
C	0.8831	0.4566	0.5434
C	0.6202	0.6064	0.4166
C	0.8836	0.5506	0.5737
C	0.6173	0.7383	0.4054
C	0.8144	0.5335	0.4087
C	0.6848	0.3919	0.5367
C	0.7903	0.4310	0.4336
C	0.7059	0.3309	0.4993
C	0.8177	0.5719	0.5969
C	0.6817	0.7998	0.3894
C	0.9674	0.7095	0.5391
C	0.9238	0.6713	0.5717
C	0.8972	0.4679	0.4740
C	0.8308	0.4003	0.4670
C	0.0164	0.1054	0.4894
C	0.4651	0.1588	0.5285
C	0.0772	0.0667	0.5495
C	0.4390	0.9718	0.4878
C	0.1168	0.9580	0.4560
C	0.3804	0.1026	0.5828
C	0.1160	0.0468	0.4253
C	0.3823	0.2342	0.5936
C	0.1853	0.0312	0.5902
C	0.3162	0.8897	0.4629
C	0.2099	0.9287	0.5649

C	0.2964	0.8226	0.4997
C	0.1816	0.0687	0.4024
C	0.3179	0.2962	0.6095
C	0.0356	0.2053	0.4602
C	0.0757	0.1683	0.4273
C	0.1012	0.9647	0.5253
C	0.1659	0.8917	0.5323
C	0.5150	0.6086	0.5096
C	0.9649	0.6630	0.4708
C	0.5791	0.5714	0.4499
C	0.9383	0.4716	0.5113
C	0.6169	0.4566	0.5434
C	0.8798	0.6065	0.4167
C	0.6163	0.5506	0.5737
C	0.8827	0.7383	0.4054
C	0.6856	0.5335	0.4087
C	0.8152	0.3919	0.5367
C	0.7098	0.4310	0.4336
C	0.7941	0.3309	0.4993
C	0.6822	0.5719	0.5969
C	0.8183	0.7998	0.3894
C	0.5326	0.7094	0.5390
C	0.5762	0.6712	0.5716
C	0.6028	0.4679	0.4740
C	0.6693	0.4003	0.4670
C	0.4836	0.1053	0.4894
C	0.0349	0.1588	0.5285
C	0.4228	0.0667	0.5495
C	0.0610	0.9719	0.4878
C	0.3832	0.9580	0.4560
C	0.1196	0.1026	0.5828
C	0.3840	0.0468	0.4253
C	0.1177	0.2343	0.5936
C	0.3147	0.0312	0.5902
C	0.1838	0.8897	0.4629
C	0.2901	0.9287	0.5649
C	0.2036	0.8226	0.4997
C	0.3184	0.0687	0.4024
C	0.1821	0.2962	0.6095
C	0.4644	0.2052	0.4601
C	0.4243	0.1683	0.4272
C	0.3988	0.9647	0.5253
C	0.3341	0.8917	0.5323
C	0.4850	0.3914	0.5096

C	0.0351	0.3370	0.4707
C	0.4210	0.4285	0.4499
C	0.0617	0.5284	0.5113
C	0.3831	0.5434	0.5434
C	0.1202	0.3935	0.4166
C	0.3837	0.4494	0.5737
C	0.1173	0.2617	0.4054
C	0.3144	0.4665	0.4087
C	0.1849	0.6081	0.5367
C	0.2903	0.5690	0.4336
C	0.2059	0.6691	0.4993
C	0.3178	0.4281	0.5969
C	0.1817	0.2002	0.3894
C	0.4674	0.2905	0.5390
C	0.4238	0.3287	0.5716
C	0.3972	0.5320	0.4740
C	0.3308	0.5997	0.4670
C	0.5164	0.8946	0.4894
C	0.9651	0.8413	0.5285
C	0.5772	0.9333	0.5495
C	0.9390	0.0282	0.4878
C	0.6168	0.0420	0.4560
C	0.8803	0.8974	0.5828
C	0.6160	0.9532	0.4253
C	0.8823	0.7658	0.5937
C	0.6853	0.9688	0.5902
C	0.8162	0.1103	0.4629
C	0.7098	0.0713	0.5649
C	0.7964	0.1774	0.4997
C	0.6816	0.9313	0.4024
C	0.8179	0.7038	0.6095
C	0.5356	0.7947	0.4602
C	0.5757	0.8317	0.4273
C	0.6012	0.0353	0.5253
C	0.6659	0.1083	0.5323
C	0.7500	0.0852	0.4412
C	0.7500	0.9076	0.6061
C	0.7500	0.9955	0.4103
C	0.7500	0.7731	0.6149
C	0.2500	0.9148	0.4412
C	0.2500	0.0924	0.6061
C	0.2500	0.0045	0.4103
C	0.2500	0.2269	0.6149
C	0.2500	0.5871	0.5591

C	0.2500	0.4048	0.3926
C	0.2500	0.4941	0.5897
C	0.2500	0.2695	0.3844
C	0.7500	0.4129	0.5591
C	0.7500	0.5952	0.3926
C	0.7500	0.5059	0.5897
C	0.7500	0.7305	0.3844
Sc	0.1512	0.3444	0.5125
Sc	0.8488	0.6556	0.5125
Sc	0.6511	0.6557	0.5125
Sc	0.3489	0.3443	0.5125
Sc	0.7500	0.9526	0.5070
Sc	0.2500	0.0474	0.5069
N	0.2500	0.2454	0.5082
N	0.7500	0.7546	0.5082

α'-$Sc_3N@C_{80}$-2D network with a =17.76 Å, b = 30.55 Å, c = 20.50 Å, α = 90°, β = 150°, γ = 90°

	x	y	z
C	0.6209	0.4870	0.2639
C	0.6209	0.5130	0.7639
C	0.9108	0.5099	0.2664
C	0.9108	0.4901	0.7664
C	0.1244	0.5354	0.7153
C	0.1244	0.4646	0.2153
C	0.3051	0.4674	0.7166
C	0.3051	0.5326	0.2166
C	0.6451	0.5558	0.3268
C	0.6451	0.4442	0.8268
C	0.0111	0.4414	0.3291
C	0.0111	0.5585	0.8291
C	0.9102	0.4886	0.6892
C	0.9103	0.5114	0.1892
C	0.4592	0.5143	0.6862
C	0.4592	0.4857	0.1862
C	0.5707	0.4491	0.3671
C	0.5707	0.5509	0.8671
C	0.1591	0.5494	0.3651
C	0.1591	0.4506	0.8651
C	0.9802	0.5962	0.6282
C	0.9802	0.4038	0.1282
C	0.2876	0.4022	0.6372
C	0.2876	0.5978	0.1372
C	0.6648	0.4144	0.3676

C	0.6648	0.5856	0.8676
C	0.0663	0.5848	0.3630
C	0.0663	0.4152	0.8630
C	0.1153	0.6084	0.6288
C	0.1153	0.3916	0.1288
C	0.1557	0.3887	0.6412
C	0.1557	0.6113	0.1412
C	0.7126	0.6039	0.4326
C	0.7126	0.3961	0.9326
C	0.1575	0.3948	0.4370
C	0.1575	0.6052	0.9370
C	0.7062	0.4583	0.5679
C	0.7062	0.5417	0.0679
C	0.4208	0.5428	0.5641
C	0.4208	0.4572	0.0641
C	0.6355	0.5754	0.4581
C	0.6355	0.4246	0.9581
C	0.2829	0.4240	0.4611
C	0.2829	0.5760	0.9611
C	0.6212	0.5009	0.5456
C	0.6212	0.4990	0.0456
C	0.4642	0.5001	0.5442
C	0.4642	0.4999	0.0442
C	0.7524	0.3878	0.4338
C	0.7524	0.6122	0.9338
C	0.1092	0.6117	0.4279
C	0.1092	0.3883	0.9279
C	0.1150	0.6279	0.5650
C	0.1150	0.3721	0.0650
C	0.0257	0.3739	0.5723
C	0.0257	0.6261	0.0723
C	0.7400	0.4533	0.2825
C	0.7400	0.5467	0.7825
C	0.8284	0.5435	0.2843
C	0.8284	0.4565	0.7843
C	0.7462	0.4163	0.3268
C	0.7462	0.5837	0.8268
C	0.9043	0.5819	0.3229
C	0.9043	0.4181	0.8229
C	0.5649	0.5285	0.3511
C	0.5649	0.4715	0.8511
C	0.1388	0.4689	0.3521
C	0.1388	0.5311	0.8521
C	0.5640	0.5370	0.4180

C	0.5640	0.4630	0.9180
C	0.2726	0.4618	0.4181
C	0.2726	0.5382	0.9181
C	0.0896	0.5096	0.2333
C	0.0896	0.4904	0.7333
C	0.3728	0.4874	0.2311
C	0.3728	0.5126	0.7311
C	0.6948	0.4683	0.7836
C	0.6948	0.5317	0.2836
C	0.8760	0.5347	0.7859
C	0.8760	0.4653	0.2859
C	0.9880	0.4408	0.1715
C	0.9880	0.5592	0.6715
C	0.3593	0.5583	0.1755
C	0.3593	0.4417	0.6755
C	0.5293	0.5146	0.8110
C	0.5293	0.4854	0.3110
C	0.0903	0.4881	0.8118
C	0.0903	0.5119	0.3118
C	0.8407	0.5482	0.1340
C	0.8407	0.4518	0.6340
C	0.4196	0.4493	0.1308
C	0.4196	0.5507	0.6308
C	0.7212	0.4056	0.8676
C	0.7212	0.5944	0.3677
C	0.0182	0.5963	0.8716
C	0.0182	0.4037	0.3716
C	0.9361	0.5828	0.1349
C	0.9361	0.4172	0.6349
C	0.3403	0.4109	0.1338
C	0.3403	0.5891	0.6338
C	0.8493	0.3924	0.8632
C	0.8493	0.6076	0.3632
C	0.8830	0.6089	0.8694
C	0.8830	0.3911	0.3694
C	0.8409	0.3950	0.0620
C	0.8409	0.6050	0.5620
C	0.2850	0.6042	0.0671
C	0.2850	0.3958	0.5671
C	0.5757	0.5423	0.9362
C	0.5757	0.4577	0.4362
C	0.2931	0.4577	0.9325
C	0.2931	0.5423	0.4325
C	0.7153	0.4237	0.0387

C	0.7153	0.5763	0.5387
C	0.3619	0.5753	0.0411
C	0.3619	0.4247	0.5411
C	0.5327	0.4997	0.9566
C	0.5327	0.5003	0.4566
C	0.3771	0.5004	0.9553
C	0.3771	0.4996	0.4553
C	0.8926	0.6095	0.0700
C	0.8926	0.3905	0.5700
C	0.2542	0.3834	0.0670
C	0.2542	0.6166	0.5670
C	0.9749	0.3733	0.9273
C	0.9749	0.6267	0.4273
C	0.8850	0.6273	0.9340
C	0.8850	0.3727	0.4340
C	0.1742	0.5441	0.2175
C	0.1742	0.4559	0.7175
C	0.2526	0.4544	0.2106
C	0.2526	0.5457	0.7106
C	0.0987	0.5838	0.1799
C	0.0987	0.4162	0.6799
C	0.2513	0.4160	0.1703
C	0.2513	0.5841	0.6703
C	0.8604	0.4684	0.1483
C	0.8604	0.5316	0.6483
C	0.4289	0.5291	0.1471
C	0.4289	0.4709	0.6471
C	0.7260	0.4613	0.0819
C	0.7260	0.5387	0.5819
C	0.4342	0.5371	0.0819
C	0.4342	0.4629	0.5819
C	0.6646	0.5671	0.0015
C	0.6647	0.4329	0.5015
C	0.3350	0.4318	0.9984
C	0.3350	0.5682	0.4984
C	0.8392	0.3769	0.9973
C	0.8391	0.6231	0.4973
C	0.1586	0.6230	0.0015
C	0.1586	0.3770	0.5015
C	0.7556	0.6021	0.0014
C	0.7557	0.3979	0.5014
C	0.2468	0.3950	0.9976
C	0.2468	0.6050	0.4976
C	0.9738	0.3673	0.9962

C	0.9738	0.6327	0.4962
C	0.0233	0.6330	0.0015
C	0.0233	0.3670	0.5015
Sc	0.1005	0.4549	0.5819
Sc	0.1005	0.5451	0.0819
Sc	0.1418	0.5502	0.5443
Sc	0.1418	0.4498	0.0443
Sc	0.8043	0.5118	0.9002
Sc	0.8043	0.4882	0.4002
N	0.9936	0.4989	0.4958
N	0.9936	0.5011	0.9958