

Supplementary Materials

Designing C₆N₆/C₂N van der Waals heterostructures for photogenerated charge carrier separation

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S1. Cell parameters of C₆N₆/C₂N heterostructure [(2 × 2)/(√3 × √3)]

$$a = b = 14.32 \text{ \AA}$$

$$c = 20 \text{ \AA}$$

$$\alpha = \beta = 90^\circ$$

$$\gamma = 120^\circ$$

S2. Crystallographic Information File (.CIF) of C₆N₆/C₂N heterostructure

N1	0.0956899970000009	0.2041299939999988	0.4399499889999987
N2	0.0956600009999988	0.3704000119999975	0.4478499889999981
N3	0.2620800139999986	0.3704000119999975	0.4476400020000000
N4	0.3731999990000006	0.0928300019999995	0.4478400050000033
N5	0.2069800049999984	0.0928800029999977	0.4397099910000009
N6	0.3732100129999978	0.2592400010000020	0.4478400050000033
N7	0.5956900119999986	0.2040300070000001	0.4525899890000034
N8	0.5957000260000029	0.3705799880000029	0.4528200029999994
N9	0.7622500060000021	0.3705799880000029	0.4529100060000033
N10	0.8731799720000026	0.0928599980000016	0.4403400120000001
N11	0.7069500090000034	0.0928400009999990	0.4482200149999969
N12	0.8733599780000034	0.2592700120000018	0.4478999970000004
N13	0.0956500019999993	0.7041400069999995	0.4480499920000014
N14	0.0957000029999975	0.8703399899999980	0.4399600030000030
N15	0.2620700000000014	0.8705400229999967	0.4477399889999987
N16	0.3733899890000032	0.5928800109999983	0.4526200000000031
N17	0.2068500069999999	0.5928800109999983	0.4524100120000014

N18	0.3733899890000032	0.7594299909999975	0.4526999890000027
N19	0.5957999829999991	0.7041299939999988	0.4483200009999990
N20	0.5957900289999998	0.8705400229999967	0.4482299980000022
N21	0.7619500160000001	0.8703600170000030	0.4406499859999968
N22	0.8733699920000007	0.5929800270000030	0.4481700059999980
N23	0.7069600219999970	0.5929899810000023	0.4484899939999991
N24	0.8731700180000033	0.7590799930000003	0.4403299989999994
N25	0.2107599969999967	0.4291499850000022	0.6049500109999997
N26	0.1012799960000024	0.5393599869999974	0.6041399839999997
N27	0.0977199969999987	0.2029500009999978	0.6185700300000008
N28	0.2079000029999989	0.0927399990000026	0.6183999779999994
N29	0.5443699960000004	0.0963200030000024	0.6042600270000023
N30	0.4341599939999981	0.2058099959999993	0.6050199869999986
N31	0.2107799950000029	0.7590600249999966	0.6049600240000004
N32	0.4304899870000014	0.8685399889999985	0.6043599839999985
N33	0.0977500010000014	0.8723700050000005	0.6186000109999981
N34	0.5407400129999971	0.7591000199999982	0.6054999830000014
N35	0.5443699960000004	0.4255099889999983	0.6045399899999992
N36	0.7671499850000032	0.8723999859999978	0.6192600130000017
N37	0.7640500070000016	0.5357300040000013	0.6054999830000014
N38	0.4304899870000014	0.5394099949999998	0.6044800279999976
N39	0.8734999899999991	0.4254800080000010	0.6044300200000023
N40	0.8773400190000018	0.0927999990000004	0.6189900039999969
N41	0.7640600200000023	0.2057799990000007	0.6052100060000001
N42	0.8773699999999991	0.7621799710000019	0.6190999749999975
C1	0.0459299979999983	0.2624000010000032	0.4432800109999988
C2	0.2039400040000032	0.4205299910000022	0.4491600099999999
C3	0.2037599980000024	0.2623899880000025	0.4431099889999999
C4	0.2652199859999982	0.0430999989999989	0.4431200029999971
C5	0.2652300000000025	0.2009299990000031	0.4431000049999980
C6	0.4233300089999972	0.2011100049999968	0.4492900070000019
C7	0.5459899900000025	0.2624500100000020	0.4526700079999983
C8	0.7038300039999967	0.4202800099999990	0.4529300029999987
C9	0.7038199899999995	0.2624500100000020	0.4527699949999970
C10	0.7651799920000002	0.0431100019999988	0.4436799879999995
C11	0.7651100160000013	0.2011200040000034	0.4494900110000017
C12	0.9229999780000000	0.2009399980000026	0.4434100089999973
C13	0.0459299979999983	0.7623500230000033	0.4433999959999966
C14	0.2037599980000024	0.9201800230000003	0.4431599970000022

C15	0.2039400040000032	0.7622900009999967	0.4492799940000012
C16	0.2652800079999977	0.5431799890000022	0.4524900019999976
C17	0.2652699949999970	0.7009999750000020	0.4525499940000017
C18	0.4230900109999993	0.7009999750000020	0.4527499969999980
C19	0.5456900000000005	0.7622900009999967	0.4496600029999982
C20	0.7037199740000020	0.9201800230000003	0.4437800050000007
C21	0.7037199740000020	0.7623500230000033	0.4438500110000021
C22	0.7651200290000020	0.5428799990000002	0.4497399930000014
C23	0.7651799920000002	0.7008799910000008	0.4438000020000032
C24	0.9229999780000000	0.7008799910000008	0.4435499909999976
C25	0.0448199989999978	0.5902799959999996	0.6048600080000028
C26	0.0463799979999990	0.7650200129999973	0.6152099970000009
C27	0.0448100010000019	0.4319800139999970	0.6048099989999969
C28	0.0463499990000003	0.2588900029999976	0.6151400210000020
C29	0.1034699980000013	0.3732500079999994	0.6083899739999978
C30	0.1034900020000009	0.7077000139999967	0.6084399820000002
C31	0.2049999979999981	0.2588900029999976	0.6150199770000029
C32	0.3782599869999999	0.2572399969999992	0.6084300280000008
C33	0.3795700069999981	0.4320299919999968	0.6049399970000024
C34	0.3782599869999999	0.0985099970000007	0.6083400249999968
C35	0.4370000059999981	0.0398500000000013	0.6047899719999990
C36	0.2638700010000008	0.0413799990000001	0.6149500009999969
C37	0.2638500030000017	0.2000299990000016	0.6149899959999985
C38	0.4370000059999981	0.3745999929999968	0.6049799919999970
C39	0.2621999979999998	0.3732700050000020	0.6083800199999985
C40	0.7126899960000017	0.0985099970000007	0.6086999770000006
C41	0.7699999809999980	0.0414099990000025	0.6155199999999965
C42	0.5952900050000025	0.0398500000000013	0.6050299999999993
C43	0.3795799909999999	0.9250100260000025	0.6048200130000012
C44	0.2622199950000024	0.8664100169999998	0.6083499790000033
C45	0.5378800029999979	0.9250199789999982	0.6050999759999982
C46	0.7111600039999999	0.9236999749999981	0.6156399850000014
C47	0.7111600039999999	0.7650499940000017	0.6157299879999982
C48	0.5378699899999972	0.5903199910000012	0.6052700279999996
C49	0.7126899960000017	0.5916900040000002	0.6089800000000025
C50	0.7700200080000030	0.7061899899999986	0.6157000059999973
C51	0.5966799859999981	0.7077299950000011	0.6089699859999982
C52	0.5952900050000025	0.5328999760000031	0.6053000089999969
C53	0.5966799859999981	0.8664600250000021	0.6088899969999986

C54	0.8714100119999983	0.5916699770000022	0.6087800259999980
C55	0.9299700259999995	0.3745799960000014	0.6049399970000024
C56	0.9286500219999994	0.2000499959999971	0.6153100129999984
C57	0.9299799799999988	0.5328599810000014	0.6050199869999986
C58	0.9286699889999994	0.7061700220000020	0.6154400109999969
C59	0.8713999989999976	0.2572300140000010	0.6086000199999972
C60	0.2050299940000002	0.9236699940000008	0.6150000100000028

S3. AIMD plot of C_6N_6/C_2N heterostructures

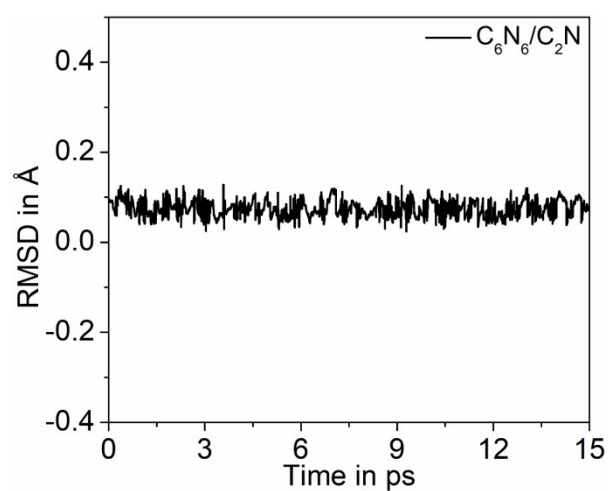


Figure S1. Plot of RMSD with time at 300 K for C_6N_6/C_2N heterostructure.

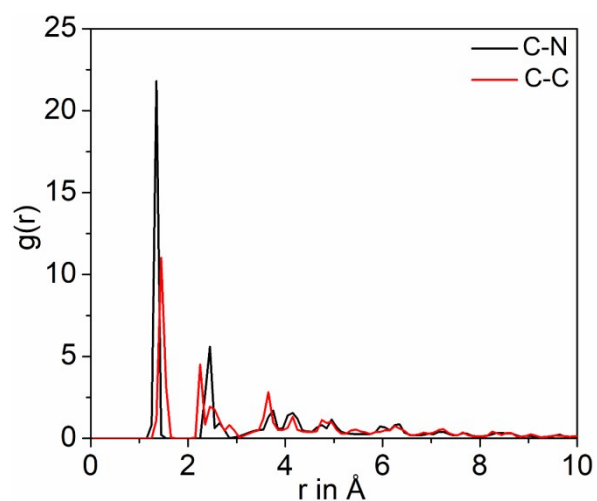


Figure S2. Plot of radial distribution function $\{g(r)\}$ between C-N pair for C_6N_6/C_2N heterostructure at 300 K.