Supplementary Material (ESI) for Chemical Communications

Ti_2C_{80} is more likely a Titanium Carbide Endohedral Metallofullerene $(Ti_2C_2)@C_{78}$

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S1 Cartesian coordinates and energies of the optimized $Ti_2@C_{80}$ and $Ti_2C_2@C_{78}$

A. $Ti_2@C_{80}$ (D_{2h}) RB3LYP/DZP optimization.

E_{tot}(Singlet) = –3164.46183 hartree; E_{tot}(triplet) = –3164.48419 au.

Coordinates:

C,0,3.0698377446,2.6713275979,0.
C,0,2.3590857601,3.1511349249,1.1678786049
C,0,3.8834237562,1.4955750296,0.
C,0,3.9160044099,0.7326342589,1.2353217325
C,0,3.0947361932,1.1569073767,2.3506122781
C,0,2.3259526995,2.3677671762,2.3591145615
C,0,2.3590857601,3.1511349249,-1.1678786049
C,0,1.2200184705,3.8765743217,0.7255087512
C,0,3.9160044099,0.7326342589,-1.2353217325
C,0,3.9160044099,-0.7326342589,1.2353217325
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C,0,3.0947361932,-1.1569073767,2.3506122781
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C,0,-3.0947361932,1.1569073767,-2.3506122781
C,0,-1.1593558605,-2.3991297223,-3.1609198864
C,0,-1.2200184705,-3.8765743217,0.7255087512
C,0,-2.6379846753,0.,-3.0605242098
C,0,-3.9160044099,0.7326342589,-1.2353217325
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C,0,-2.3590857601,-3.1511349249,1.1678786049
C,0,-2.3259526995,-2.3677671762,-2.3591145615
C,0,-3.0947361932,-1.1569073767,-2.3506122781
C,0,-3.9160044099,-0.7326342589,-1.2353217325
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Ti,0,-2.2506033191,0.,0.
Ti,0,2.2506033191,0.,0.

B. $Ti_2C_2@C_{78}$ (C_{2v}) RB3LYP/DZP optimization.

E_{tot}(Singlet) = −3164.43756 hartree.

Coordinates:

C,0,0.7141573092,3.951135117,1.2614543732
C,0,-0.7141573092,3.951135117,1.2614543732
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C,0,-1.4432370453,3.9685553632,0.0016799916
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C,0,-0.7307999023,4.0013437501,-1.2421736464
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C,0,-1.4133461956,3.1020660274,2.1750800546
C,0,-2.5810882684,3.1012544452,0.1484827309
C,0,1.1658218686,3.0928327488,-2.2727380872
C,0,-1.1658218686,3.0928327488,-2.2727380872
C,0,2.6067254523,2.6428429766,1.5112964771
C,0,-2.6067254523,2.6428429766,1.5112964771
C,0,0.,2.6230188632,-2.9692312778
C,0,0.7350399019,2.3081676369,3.1712528963
C,0,-0.7350399019,2.3081676369,3.1712528963
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C,0,-3.1189728056,2.3119586432,-0.9357359695
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C,0,-3.2302057081,1.4192322835,1.8718263291
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C,0,-1.4224341183,1.1623671669,3.6142075108
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C,0,2.4127518229,1.1648197324,-3.0225102256
C,0,-3.8416844622,1.1648529144,-0.5595372267
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C,0,3.8894656692,0.7088211571,0.8276922531
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C,0,-1.235240888,0.7087749277,-3.7620019015
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C,0,-0.701478258,0.,4.0387428353
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C,0,1.4224341183,-1.1623671669,3.6142075108
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C,0,-0.7307999023,-4.0013437501,-1.2421736464
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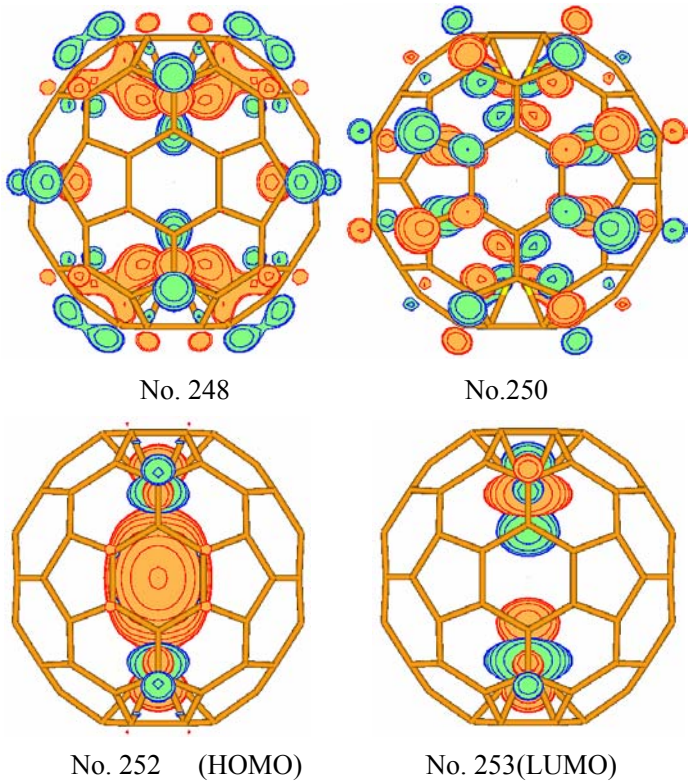

Fig. S1 Selected molecular orbitals of singlet $Ti_2@C_{80}$ (D_{2h}) that have significant contributions from the valence orbitals of Ti atoms. Note the No.252 MO is mainly localized on the Ti atoms.

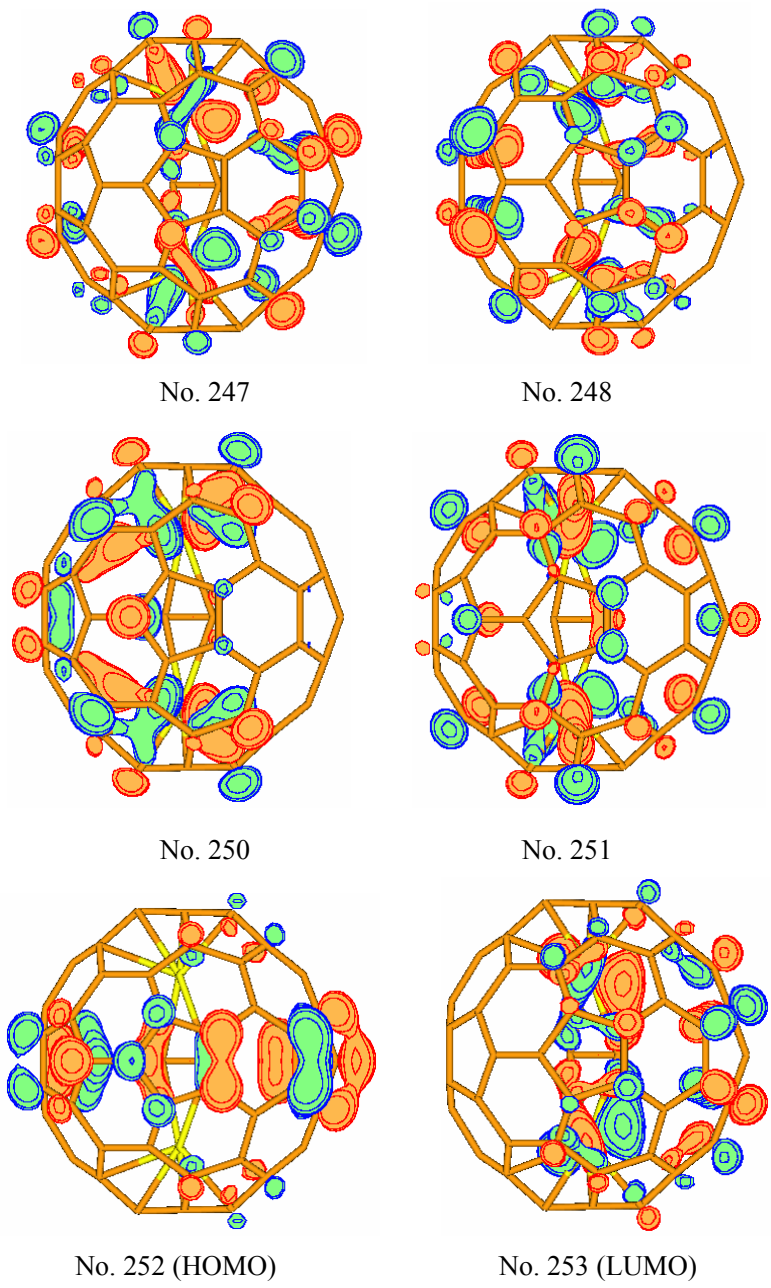

Fig. S2 Selected molecular orbitals of $Ti_2C_2@C_{78}$ (C_{2v}), among which Nos. 247, 248, 250, and 251 MOs have contributions from the valence orbitals of Ti atoms.