References where the mathematical symbols are defined:
The fragment molecular orbital method: practical applications to large molecular systems、D. G. Fedorov, K. Kitaura, Eds., CRC Press (2009), in press, chapter 1, **or**
D. G. Fedorov, K. Kitaura, J. Phys. Chem. A 111 (2007) 6904-6914

```
One-body FMO properties.
 ========================

                          E  E'_I        DX        DY        DZ
   1(frg00001,L1)    -76.368024057  -1.66667   0.62299   1.39538
   2(frg00002,L1)    -76.368062948   1.20960   1.04212  -1.58706
   3(frg00003,L1)    -76.368034599   0.35547  -1.98746  -0.99232

 Total energy of the molecule: Euncorr(1)=     -229.104121604
 Dipole moment D(xyz),DA(1)=   -0.1015993   -0.3223615   -1.1839952    1.2312936

 Energy gradient (hartree/bohr), no BSSE: G(1)

  ATOM# FRG#   Z          E'X            E'Y            E'Z
     1    1   8.0      -0.004458002     0.009078649     0.016153082
     2    1   1.0       0.006669925     0.002414628    -0.001125262
     3    1   1.0      -0.002007016    -0.011533281    -0.014309482
     4    2   8.0       0.008904604    -0.001985700    -0.018161402
     5    2   1.0      -0.001314770    -0.006772807     0.002149070
     6    2   1.0      -0.007738170     0.008626191     0.015110441
     7    3   8.0      -0.004659212    -0.012024374    -0.014849716
     8    3   1.0      -0.005265765     0.005099492     0.000260966
     9    3   1.0       0.009868405     0.007097202     0.014772303

      (1) MAXIMUM GRADIENT =  0.0181614    RMS GRADIENT = 0.0094106

 Two-body FMO properties.
 ========================

 DL: D=C dynamically correlated (MP2,CI), D=N not dynamically correlated
 (RHF,DFT). D=S separated dimer: semiclassical interaction (ES), D=M MCSCF.
 L stands for layer, Z is the monomer charge product, R is the interfragment
 distance relative to van-der-Waals radii (-1.00 is printed if distances are
 not computed). dDIJ*VIJ is the density polarisation contribution.
 Q(I->J) is the charge transfer amount, printed as zero if not available.
 Positive values correspond to I in IJ having extra negative charge.

    I    J DL  Z    R    Q(I->J)        E          EIJ-EI-EJ   dDIJ*VIJ      tot
                   R_IJ   ΔQ_IJ                    ΔE'_IJ    Tr(ΔD^IJ V^IJ)  ΔE^int_IJ
 ------------------------------------------------------------------------------------
    2    1 N1  0   0.76  0.0529   -152.749614468  -0.01352746 -0.00114287   -9.206
    3    1 N1  0   0.76 -0.0510   -152.749513638  -0.01345498 -0.00110265   -9.135
    3    2 N1  0   0.77  0.0480   -152.748428743  -0.01233120 -0.00105509   -8.400

 Total energy of the molecule: Euncorr(2)=     -229.146735861  E^FMO2-DFT
 Dipole moment D(xyz),DA(2)=   -0.1328073   -0.2992231   -1.1875491    1.2318462  D^FMO2-RHF
```

Charge transfer for each fragment:

```
 IFG QFG  DeltaQ     and its contributions from JFG, Q(JFG->IFG).
--------------------------------------------------------------------------------
   1  0   0.0018 =    2->  0.0529    3-> -0.0510
   2  0  -0.0049 =    1-> -0.0529    3->  0.0480
   3  0   0.0030 =    1->  0.0510    2-> -0.0480
```

Total absolute monomer transf. charge = 0.009705 $\Delta\overline{Q}$

Total amount of absolute transf. charge = 0.151896 ΔQ

Energy gradient (hartree/bohr), no BSSE: G(2) $\nabla E^{\text{FMO2-DFT}}$

ATOM#	FRG#	Z	E'X	E'Y	E'Z
1	1	8.0	-0.019488799	0.008990668	0.018466806
2	1	1.0	0.021271212	0.010289003	-0.002489306
3	1	1.0	-0.001319172	-0.013411622	-0.016198217
4	2	8.0	0.015231132	0.010942236	-0.021159206
5	2	1.0	-0.001515458	-0.023418078	0.004023099
6	2	1.0	-0.009188179	0.008992434	0.016733342
7	3	8.0	0.002955748	-0.024473418	-0.014059464
8	3	1.0	-0.019183837	0.013621367	-0.000778414
9	3	1.0	0.011237352	0.008467410	0.015461361

(2) MAXIMUM GRADIENT = 0.0244734 RMS GRADIENT = 0.0141661

DFT exchange+correlation energy= -22.620105871
Total electron number = 30.000119697

n-body Mulliken atomic charges Q(n)

IAT	IFG	Z	Q(1)	Q(2)	Q(3)
1	1	8.0	-0.854992	-0.831642	
2	1	1.0	0.445786	0.428840	
3	1	1.0	0.409205	0.404644	
4	2	8.0	-0.852980	-0.833508	
5	2	1.0	0.445705	0.426979	
6	2	1.0	0.407275	0.401676	
7	3	8.0	-0.853967	-0.829733	
8	3	1.0	0.446459	0.430035	
9	3	1.0	0.407508	0.402709	