Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2013

Electronic Supplementary Information for Tuning Solid-state Blue and Red Luminescence by the Formation of Solvate Crystals

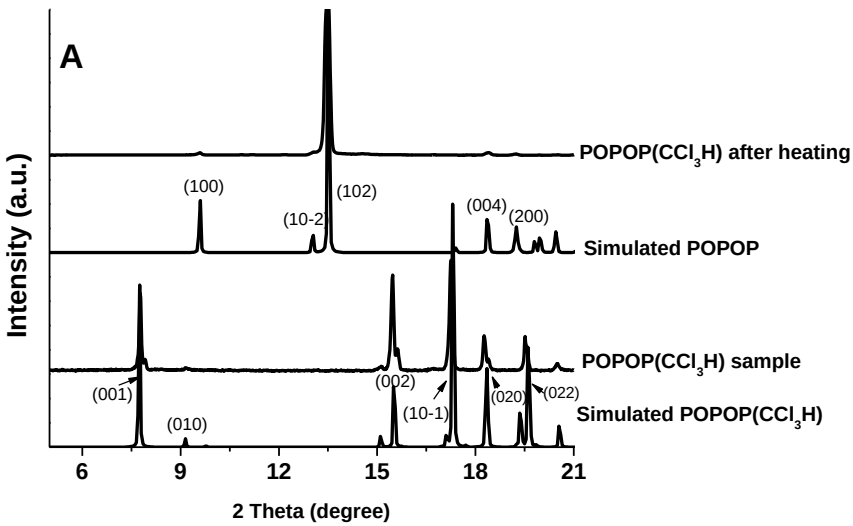
Dongpeng Yan,[a,*] Guoling Fan,[a] Yan Guan,[b] Qingyun Meng[a], Congju Li[c,d], and Jiaona Wang[c,d]

[a] *State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, P. R. China, Email: yandp@mail.buct.edu.cn*

[b] *College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, P. R. China.*

[c] *College of Material Science and Engineering, Beijing Institute of Fashion Technology, Beijing 100029, P. R. China,*

[d] *Beijing Key Laboratory of Clothing Materials R&D and Assessment, Beijing 100029, P. R. China*



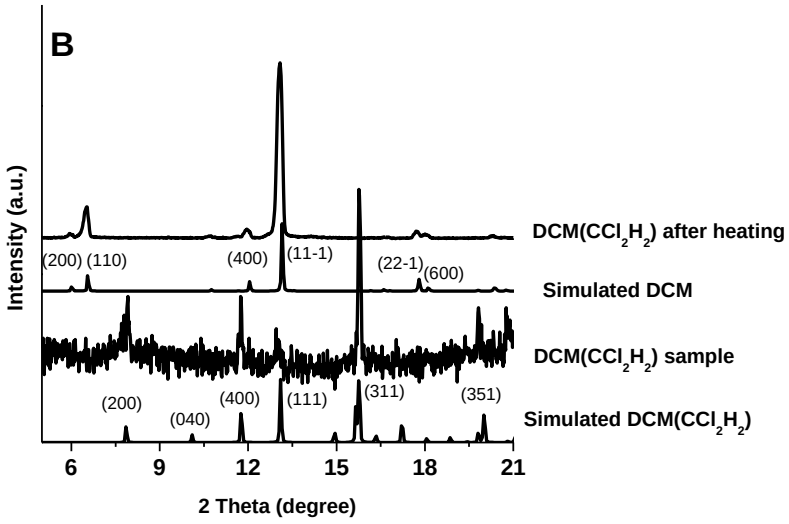


Fig. S1. Experimental and simulated XRD patterns for (A) POPOP/POPOP (CCl_3H) and (B) DCM/DCM (CCl_2H_2) before and after heating treatment.

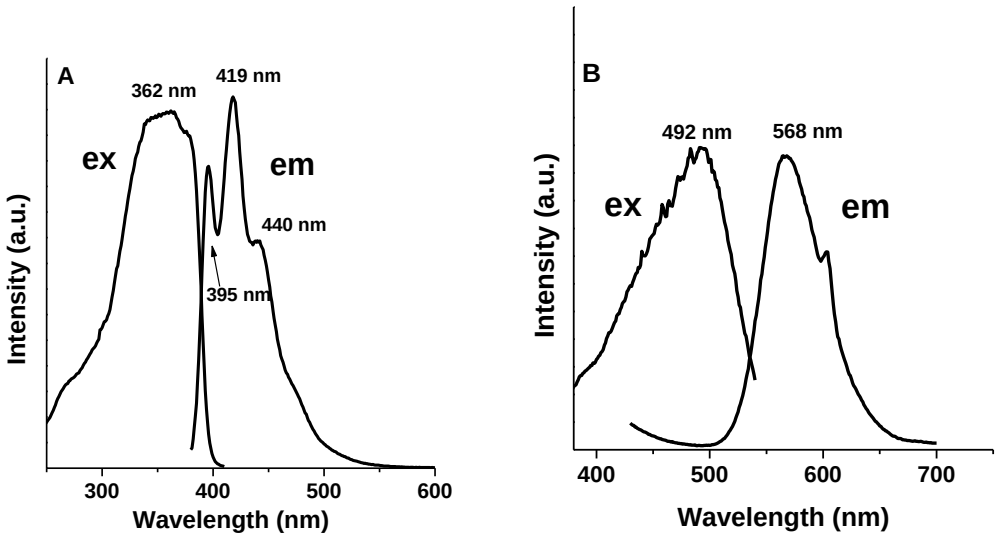


Fig. S2. Fluorescent excitation and emission spectra of POPOP (A) and DCM (B) solutions (10^{-5} mol/L) in CCl_3H and CH_2Cl_2 solvents, respectively.

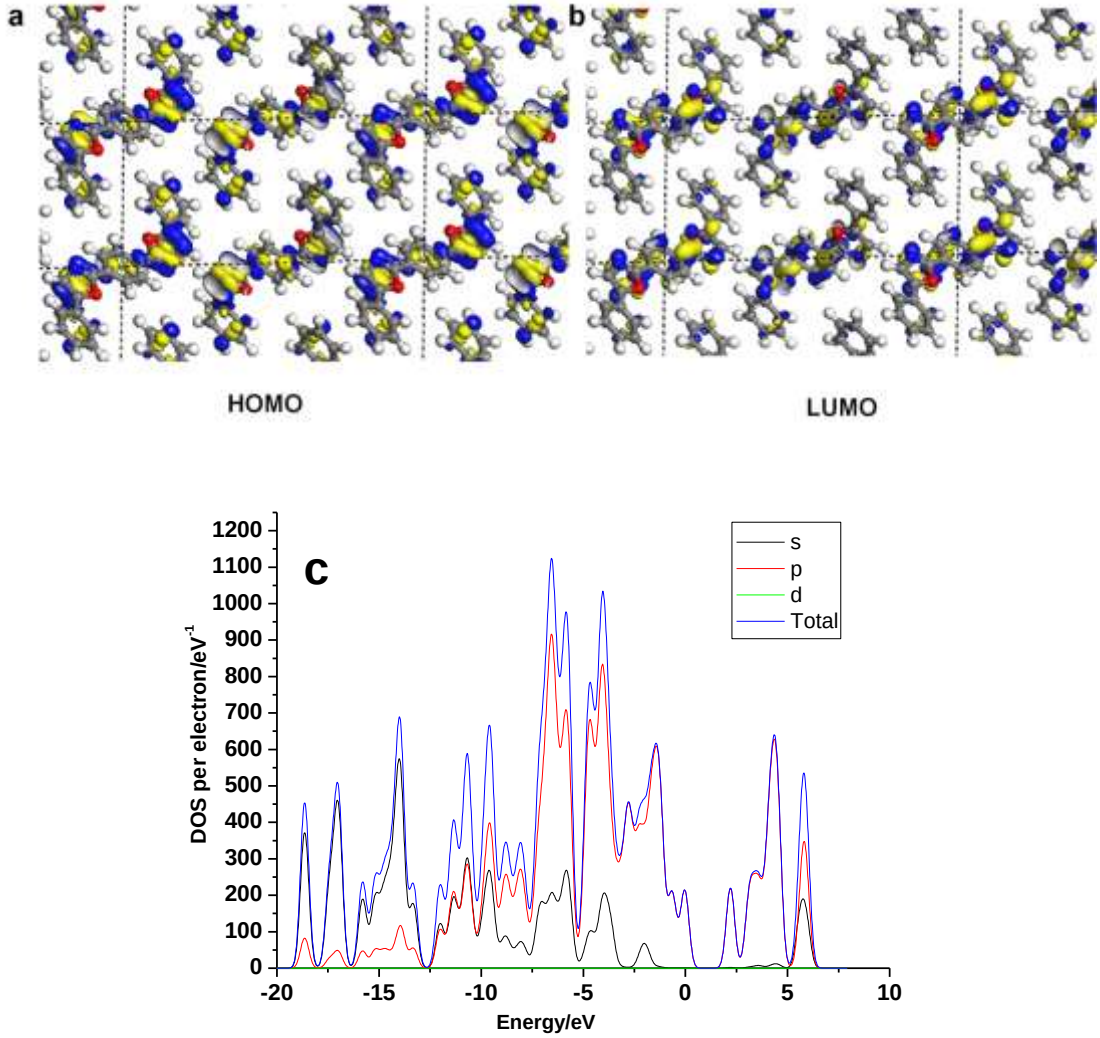
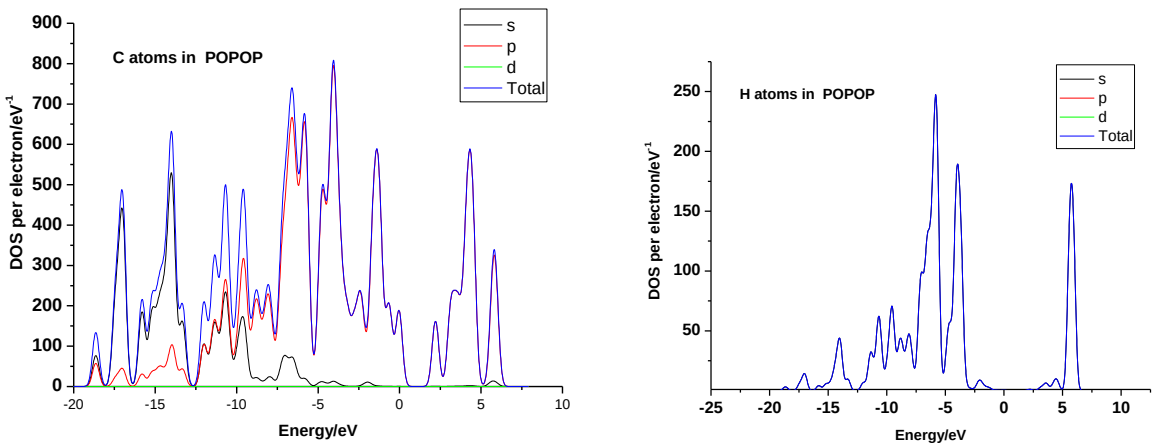


Fig. S3. a) HOMO, b) LUMO and c) total and partial electronic density of states (TDOS and PDOS) profiles for pure POPOP crystal. The Fermi energy level E_F was set to zero.



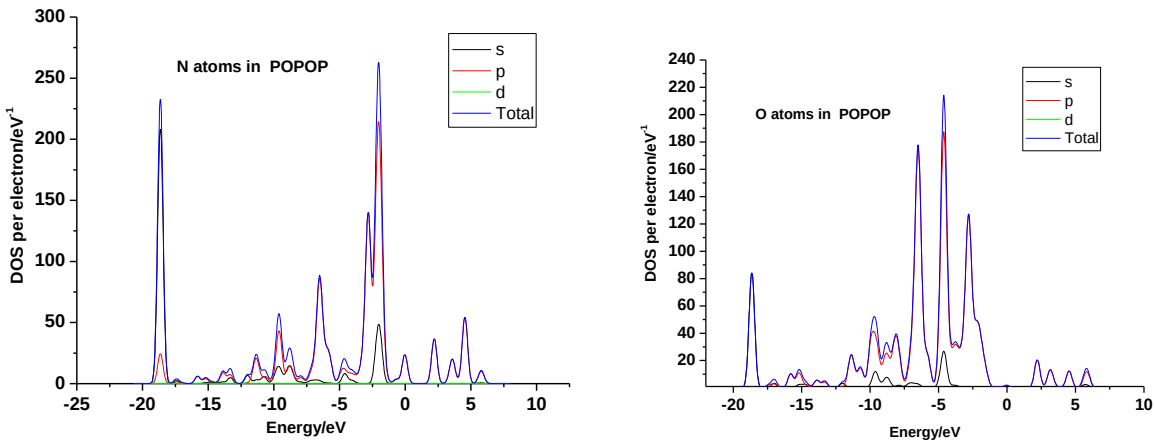
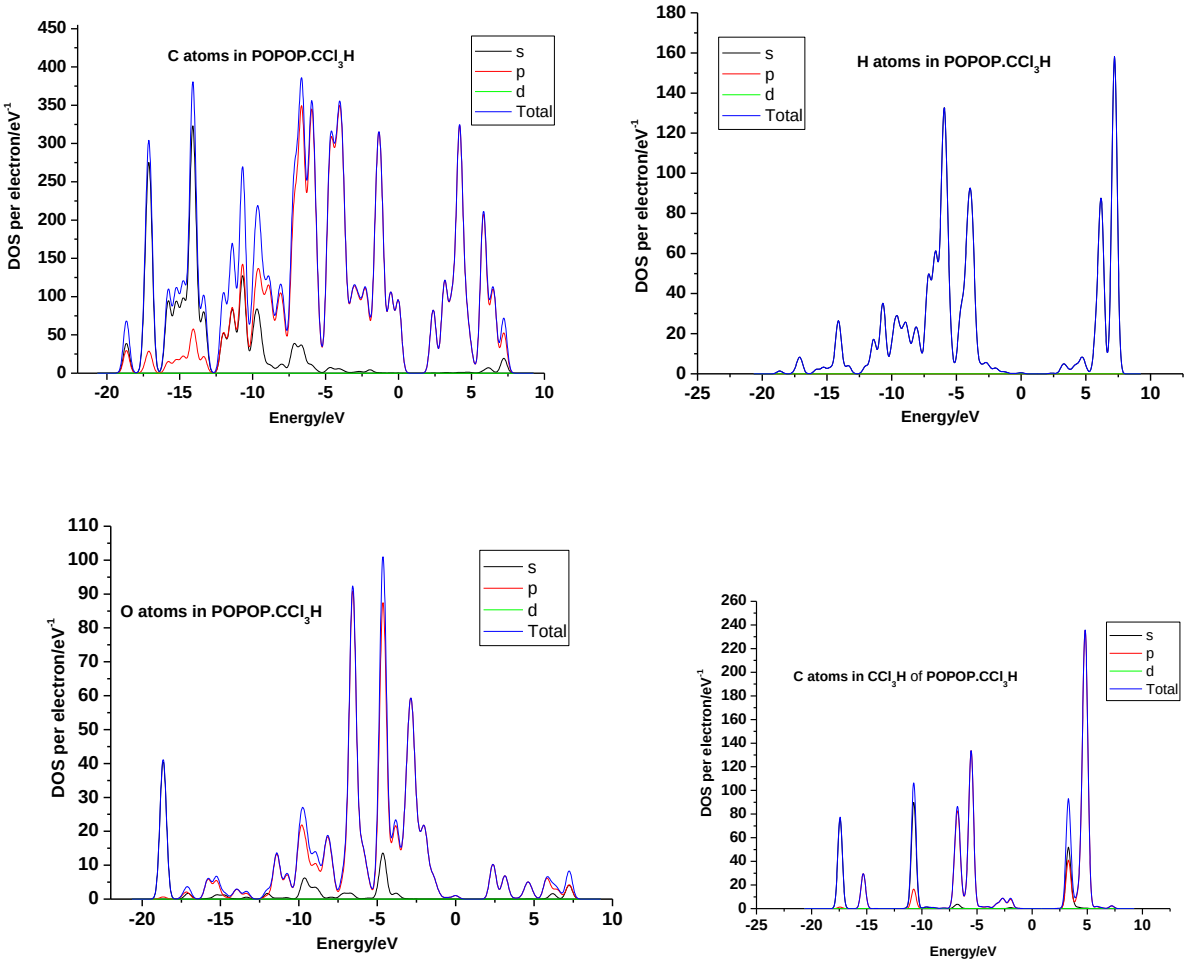


Fig. S4. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in pure POPOP crystal.



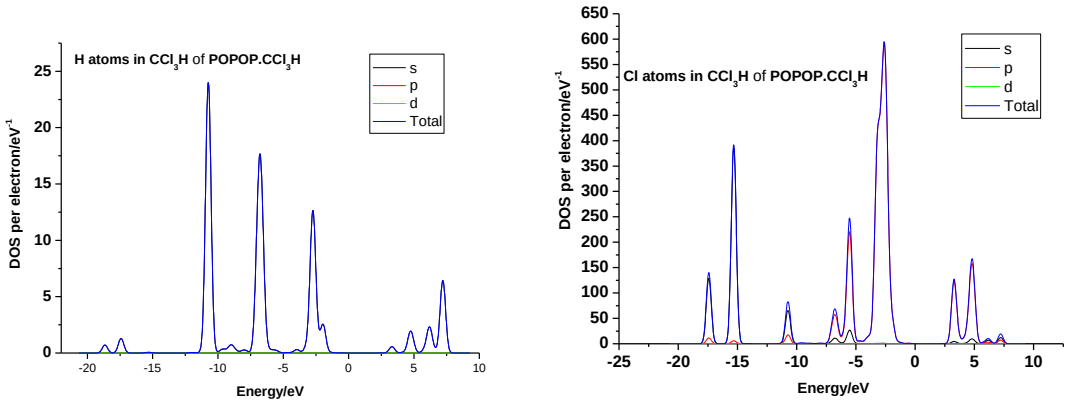


Fig. S5. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in POPOP (CCl_3H) crystal.

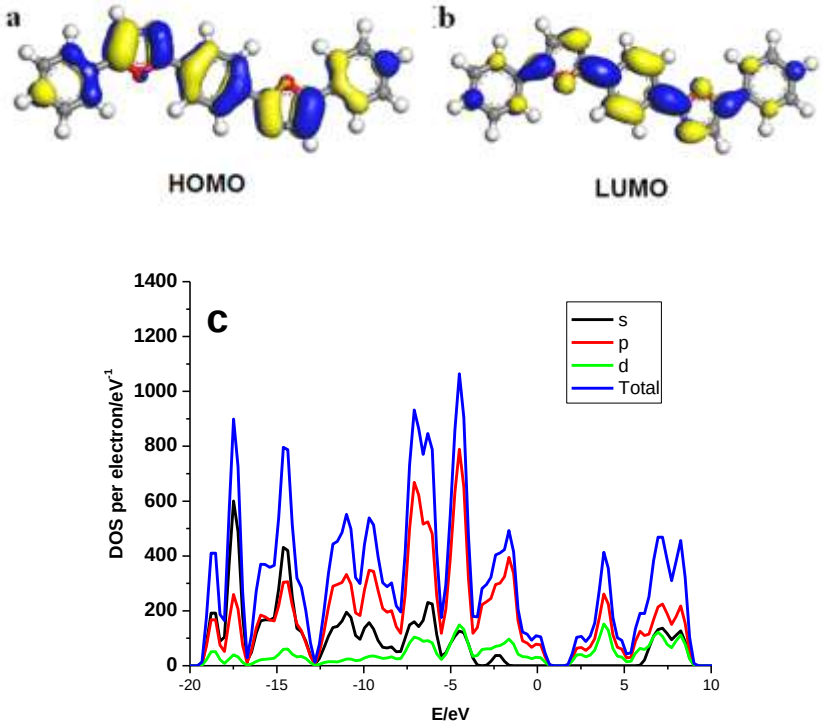


Fig. S6. a) HOMO, b) LUMO and c) total and partial electronic density of states (TDOS and PDOS) profiles for POPOP molecule (monomer state). The Fermi energy level E_F was set to zero.

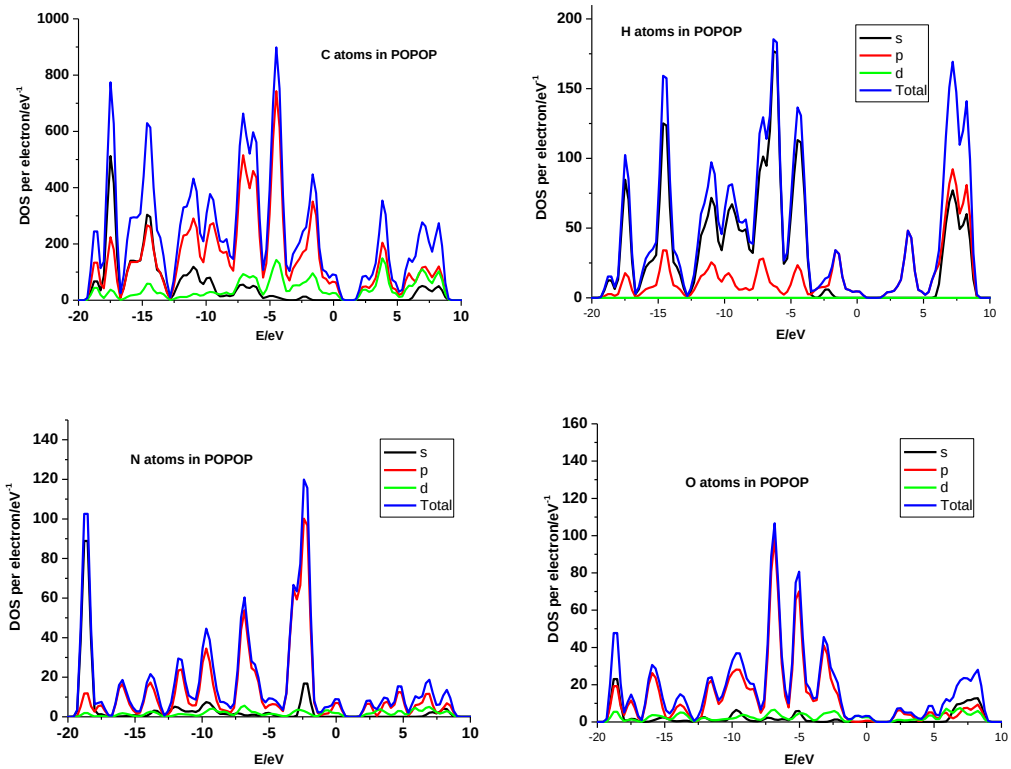
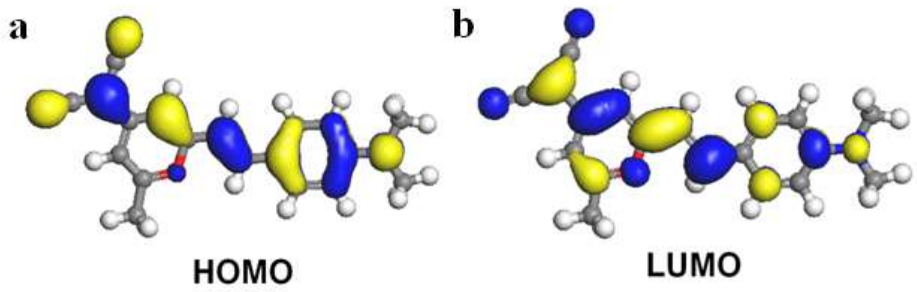


Fig. S7. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in POPOP molecule (monomer state). The Fermi energy level E_F was set to zero.

For the POPOP molecule, it can be observed that highest occupied molecular orbitals (HOMOs) are mainly populated on the C and N atoms in POPOP, while lowest unoccupied molecular orbitals (LUMOs) are located on both the C, O and N atoms in POPOP, respectively. Such behavior may suggest the photo-induced intramolecular charge transfer occurs. Near the Fermi level, the TDOS are mainly contributed by the 2p electrons of C and N atoms. The calculated energy gap is 2.71 eV, which is slightly lower than that of experimental value (2.95 eV).



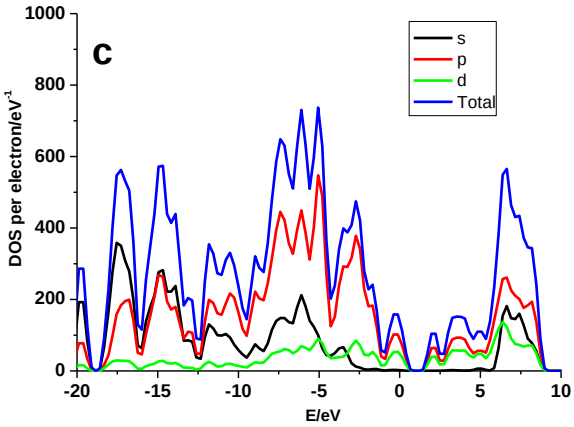


Fig. S8 a) HOMO, b) LUMO and c) total and partial electronic density of states (TDOS and PDOS) profiles for DCM molecule (monomer state). The Fermi energy level E_F was set to zero.

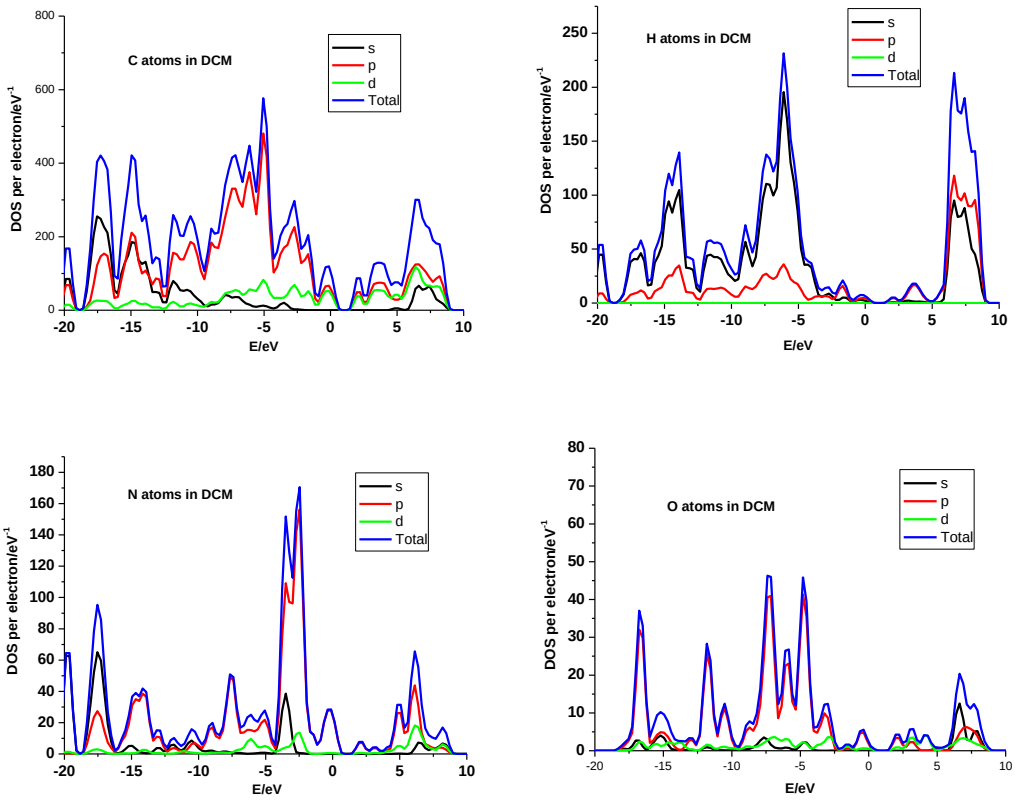


Fig. S9. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in DCM molecule (monomer state). The Fermi energy level E_F was set to zero.

For the DCM molecule system, HOMOs and LUMOs are nearly populated over the whole π-conjugated DCM molecule. The calculated energy gap is 2.10 eV, which is slightly lower than that of experimental value (2.18 eV).

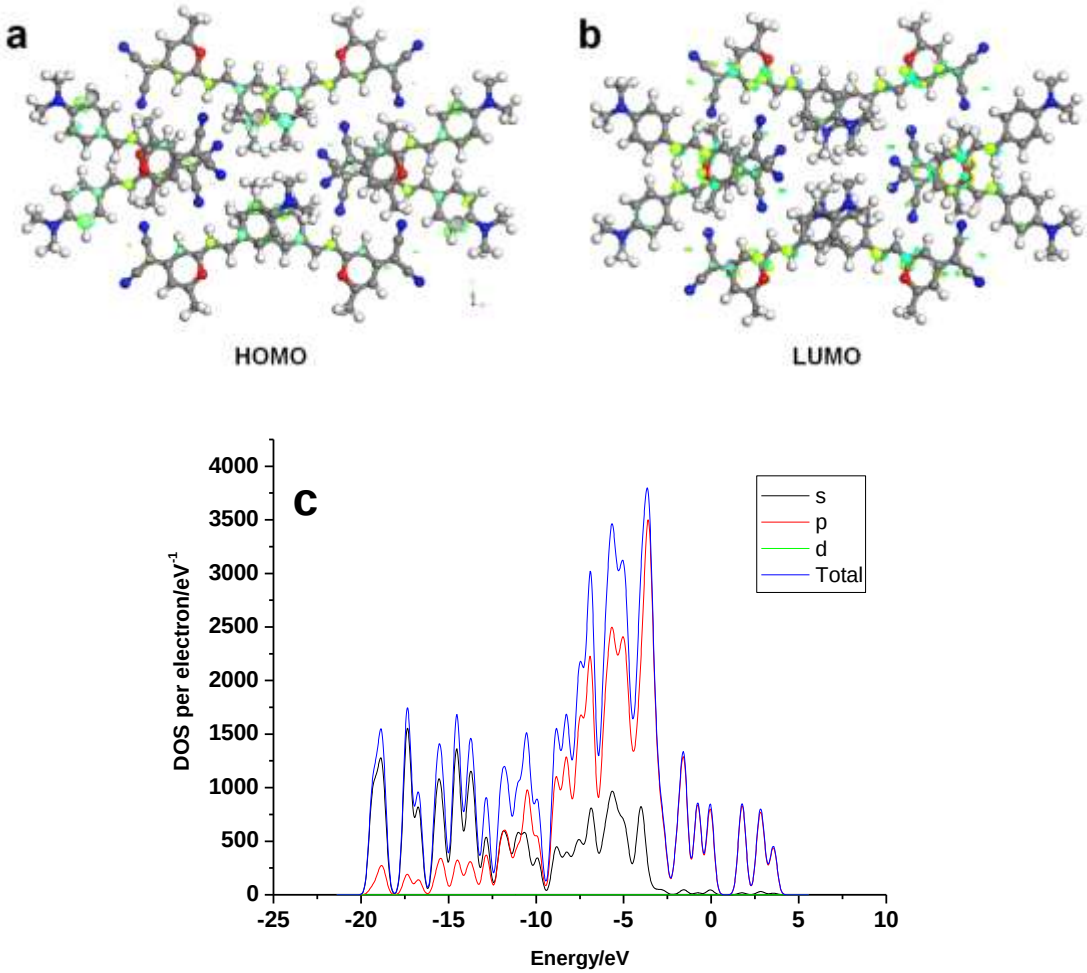
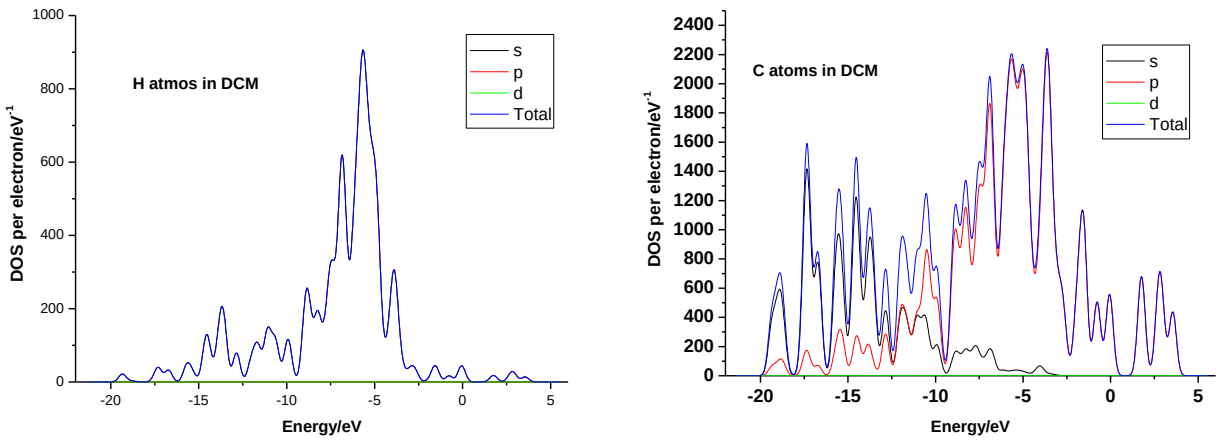


Fig. S10. a) HOMO, b) LUMO and c) total and partial electronic density of states (TDOS and PDOS) profiles for pure DCM crystal. The Fermi energy level E_F was set to zero.



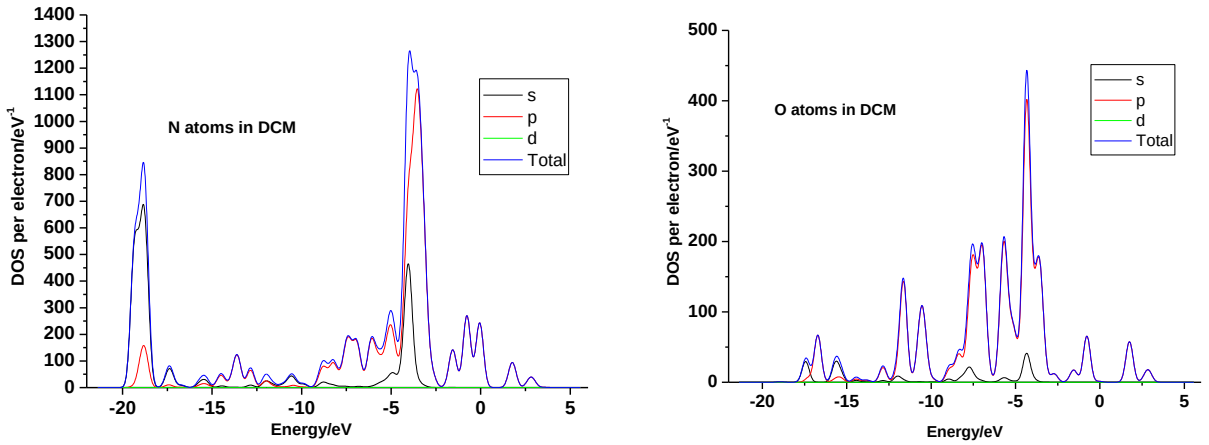
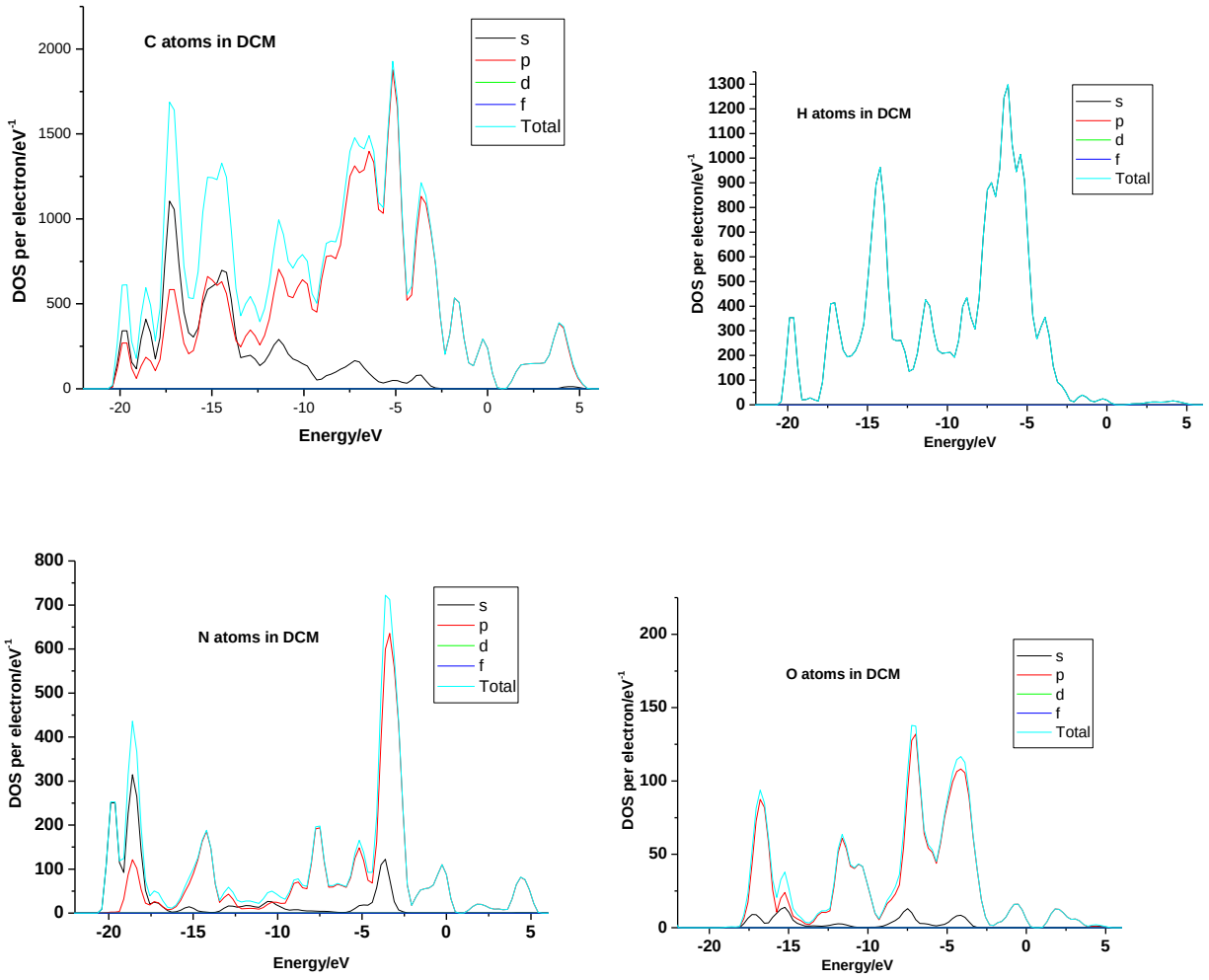


Fig. S11. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in pure DCM crystal.



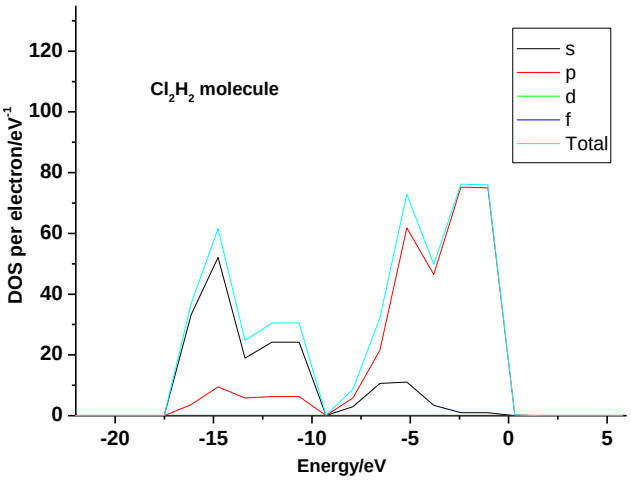


Fig. S12. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in pure DCM (CCl_2H_2) crystal.