Supplementary Information (SI) for RSC Advances.
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Supplementary information

1. Cartesian coordinates for the conformer used in all the calculations.

C	-2.843128	0.616859	-1.103441
H	-3.441060	0.369757	-1.963456
C	-2.517635	1.817416	-0.563430
N	-2.225067	-0.349070	-0.342933
C	-1.547031	0.248332	0.631866
N	-1.707511	1.563123	0.519939
H	-2.775023	2.818832	-0.861682
H	-0.906328	-0.241706	1.347556
C	-2.236549	-1.800474	-0.580642
H	-2.545104	-1.939184	-1.617491
H	-1.203238	-2.134690	-0.473240
C	-3.166777	-2.522911	0.380247
H	-4.194693	-2.161859	0.293914
H	-2.833207	-2.394963	1.412187
H	-3.156009	-3.591301	0.157343
H	-0.172464	2.082099	1.812029
C	-1.046708	2.555714	1.365011
H	-1.738138	2.914935	2.127729
H	-0.720710	3.382402	0.735512
S	1.726667	-0.629092	0.725981
O	0.696514	-1.630332	0.399287
O	3.048689	-1.133774	1.021740
C	1.918045	0.277487	-0.895700
F	0.732010	0.803329	-1.281361
F	2.326010	-0.533756	-1.867497
F	2.782314	1.284631	-0.796545
O	1.212677	0.429155	1.613978

2. Representative input file for ground state and TD-DFT calculations in MolGW

```
&molgw

 scf='LIBXC:469'
 tolscf=1.0e-10
 nscf=600
 npulay_hist=15
 init_hamiltonian='core'
 min_overlap=5e-05
 integral_quality='medium'
 grid_quality='medium'
 ecp_quality='medium'
 basis='aug-cc-pVDZ'
 auxil_basis='aug-cc-pVDZ-RI'
 postscf='td'
 triplet='no'
 frozencore='no'

 assume_scf_converged='no'
 read_restart='no'
 scf_diago_flavor='D'
```

```
 postscf_diago_flavor='D'

 xyz_file='./EMIM_OTF.xyz'
/
```