

## Description of Additional Supplementary Files:

### Supplementary Data 1:

sma\_frq:

benzene.txt

Initial excitation energies for Benzene.

butadine.txt

Initial excitation energies for Butadine.

cd33\_znpc\_znpc.txt

Initial excitation energies for Cd<sub>33</sub>Se<sub>33</sub>/Zn<sub>93</sub>S<sub>93</sub>-  
2(ZnPc).

cd33\_znpc\_znpc\_dpa.txt

Initial excitation energies for Cd<sub>33</sub>Se<sub>33</sub>/Zn<sub>93</sub>S<sub>93</sub>-  
2(ZnPc)-DPA.

f-cororene.txt

Initial excitation energies for F-cororene.

nano\_tube.txt

Initial excitation energies for Zinc-porphyrin  
molecules on a carbon nanotube.

p3b2.txt

Initial excitation energies for P3b2.

qd\_znpc.txt

Initial excitation energies for Cd<sub>38</sub>Se<sub>38</sub>-ZnPc<sub>32</sub>(NH<sub>2</sub>CH<sub>3</sub>).

qd\_znpc\_dpa.txt

Initial excitation energies for Cd<sub>38</sub>Se<sub>38</sub>-ZnPc-DPA<sub>32</sub>(NH<sub>2</sub>CH<sub>3</sub>).

ru\_tio2.txt

Initial excitation energies for Cis-[Ru(4,4'-COOH-2,2'-  
bpy)<sub>2</sub>(NCS)<sub>2</sub>] on an anatase (101).

znpc\_aggregate.txt

Initial excitation energies for Molecular ZnPc j-aggregate.

znpc\_si.txt

Initial excitation energies for ZnPc molecules on Si  
(111).