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Modulation of Chiral Spectra Deflection by Van der Waals Force-Induced Molecular Electropolarization in catenane oligomer

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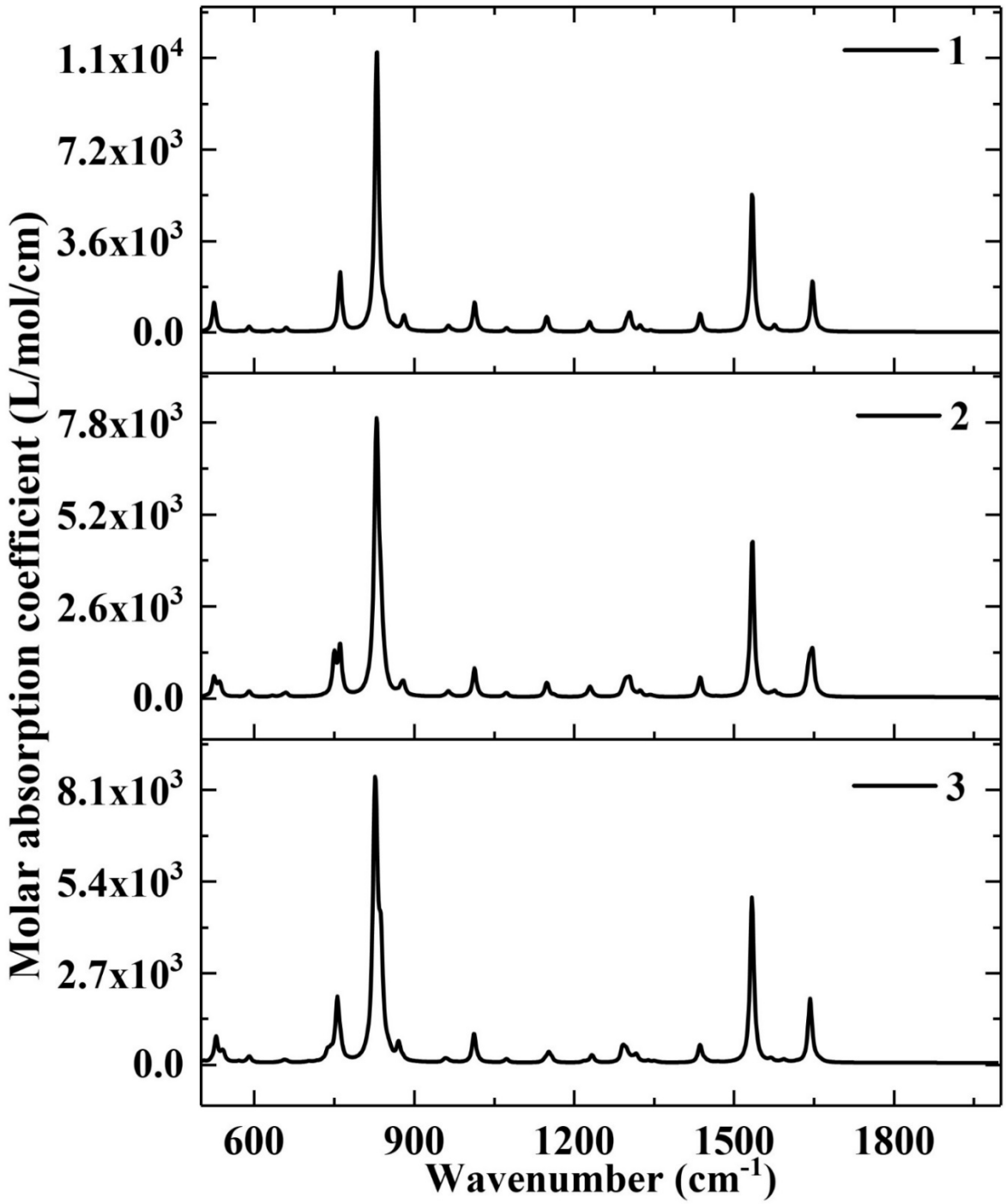

Figure S1. IR diagram of three structures.

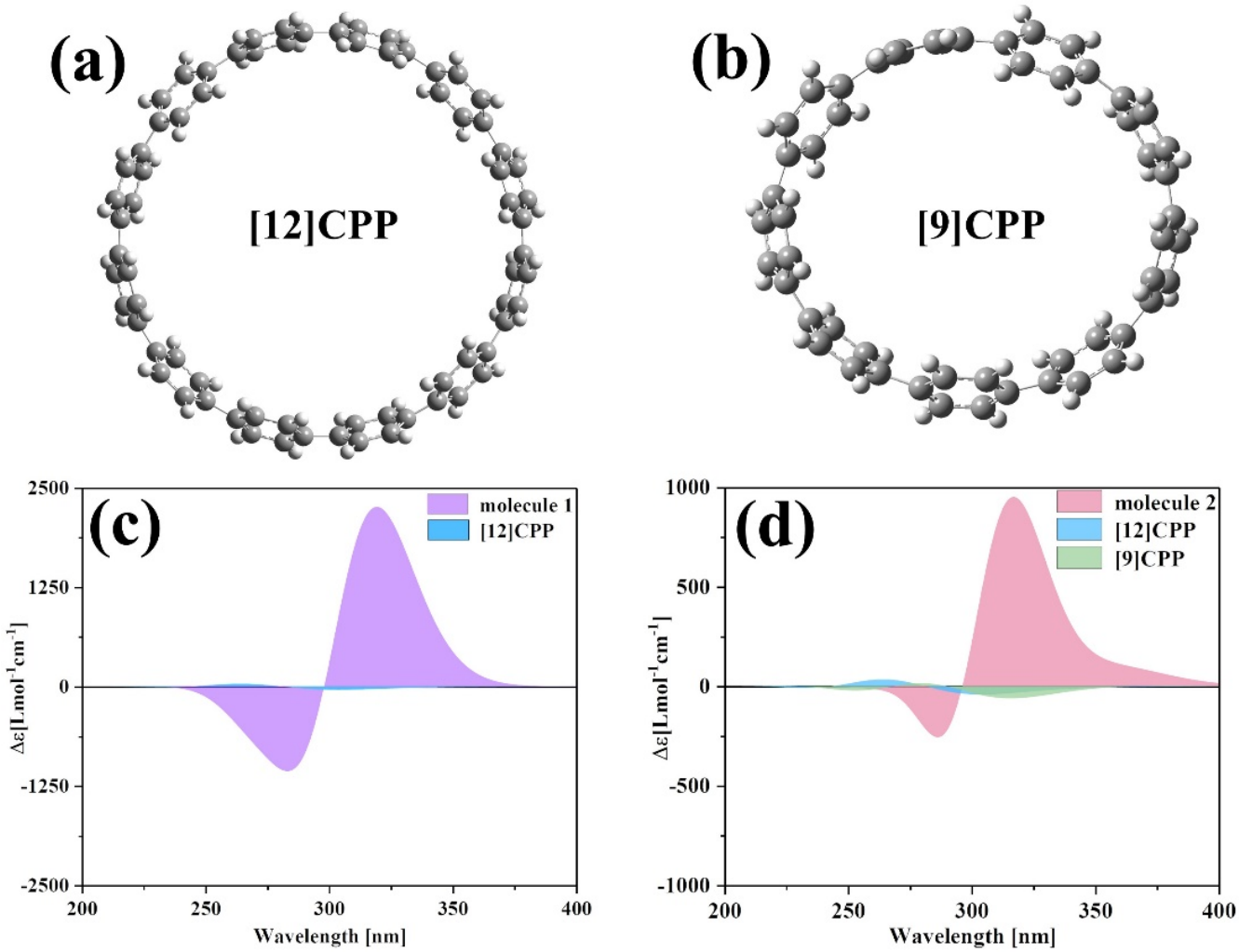

Figure S2. The structure of [12]CPP (a) and [9]CPP (b). Comparative ECD spectra of molecular 1 and [12]CPP (c). Comparative ECD spectra of molecules 2, [12]CPP and [9]CPP.

In terms of structure, [12] CPP and [9] CPP molecules can overlap with their mirrored structures, so there is no enantiomer in the molecule, which means that these two separate fragments do not have chirality. After calculation, the ECD spectra of [12] CPP and [9] CPP molecules have only very small absorption peaks, indicating that these two separate molecules have almost no chirality. However, when a new structure is formed by nesting between rings, molecule 1 and molecule 2 cannot coincide with their mirror image model, and van der Waals interactions can induce the generation of chirality. At this point, these two structures obtain strong chirality.

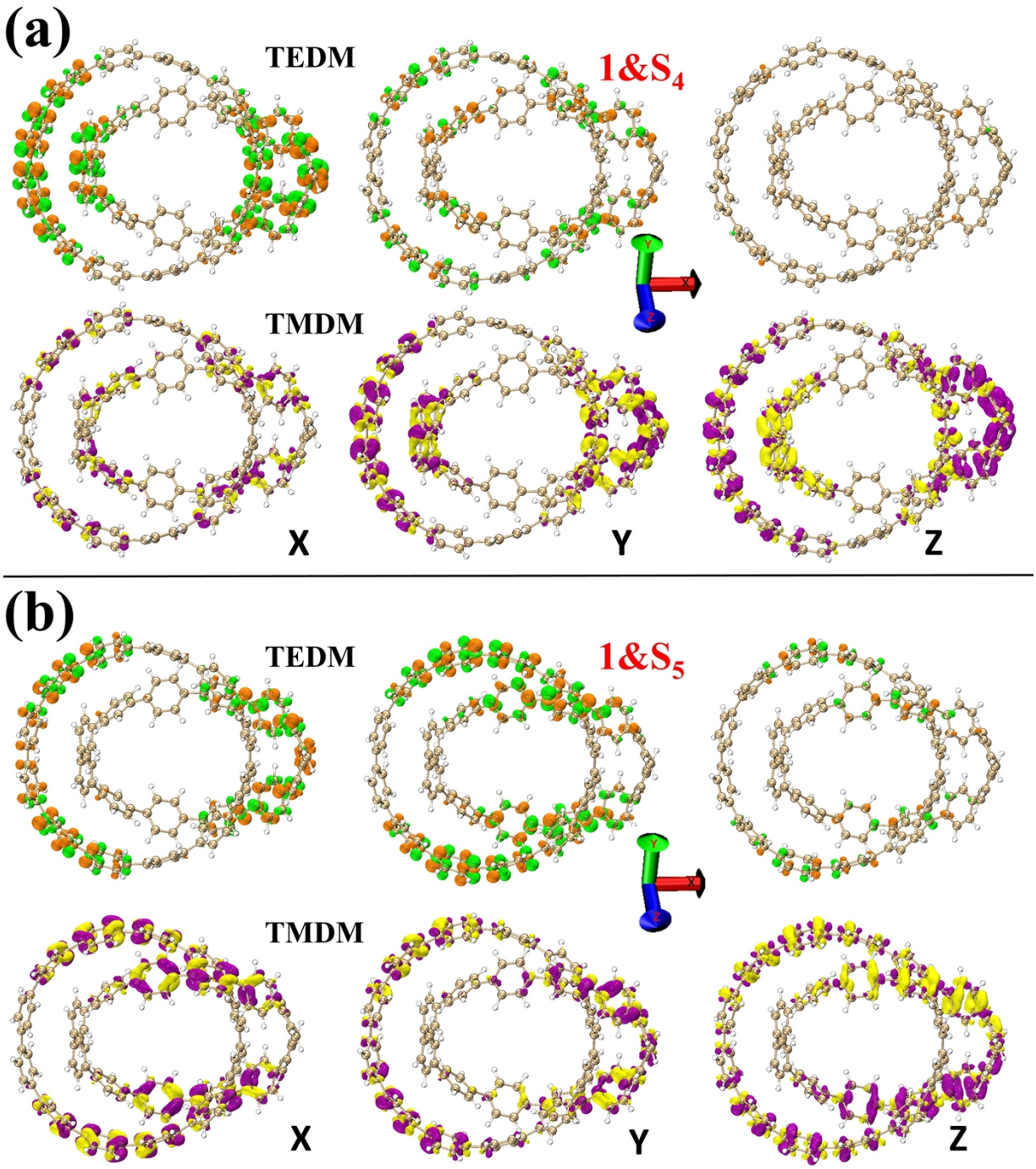

Figure S3. 1&S_4 (a), S_5 (b) are TEDMs\TMDMs in different directions. The green (orange) isosurfaces represents the positive (negative) transition electric dipole moment, and yellow (purple) isosurfaces represents the positive (negative) transition magnetic dipole moment.

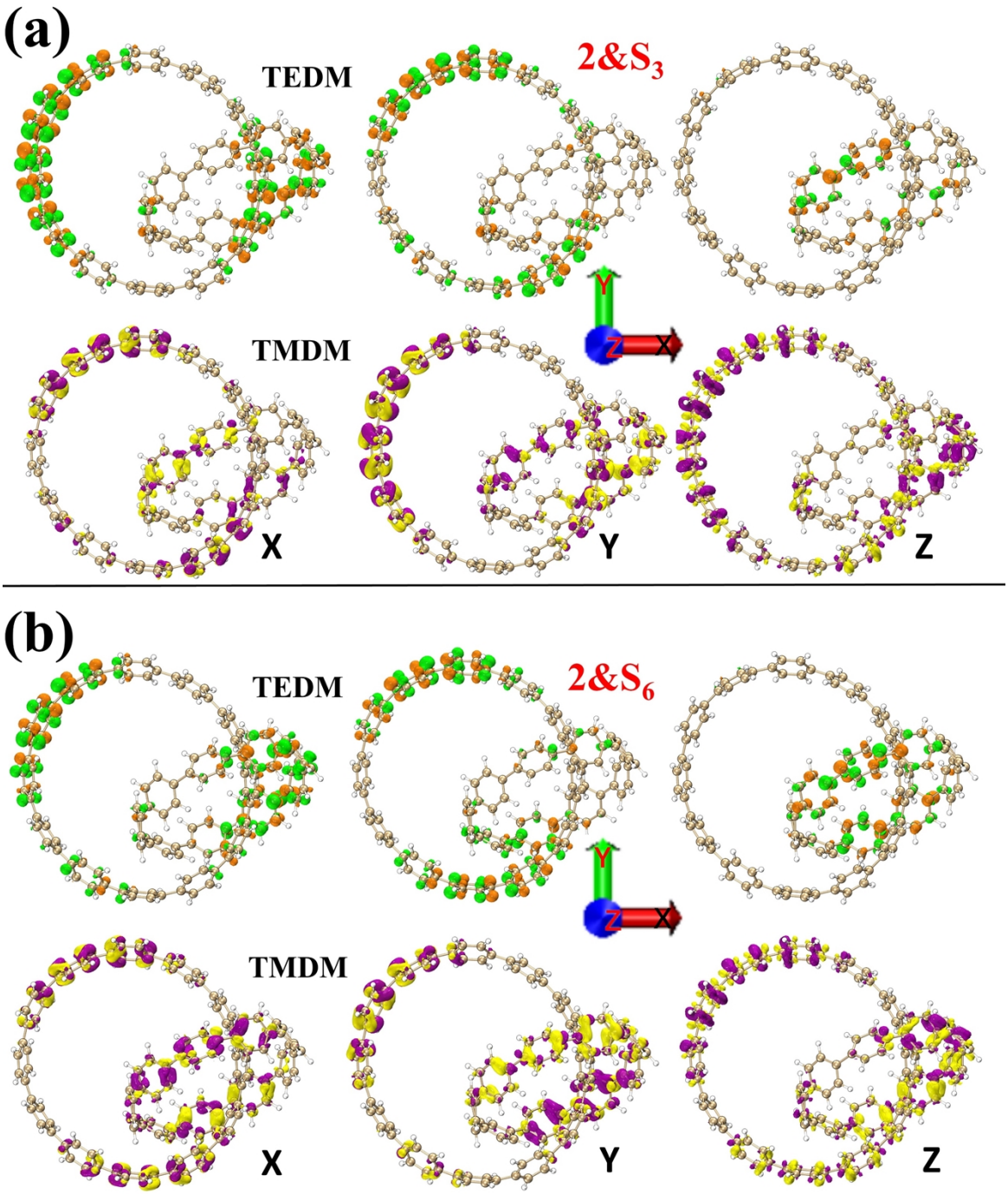

Figure S4. 2&S_3 (a), S_6 (b) are TEDMs\TMDMs in different directions. The green (orange) isosurfaces represents the positive (negative) transition electric dipole moment, and yellow (purple) isosurfaces represents the positive (negative) transition magnetic dipole moment.

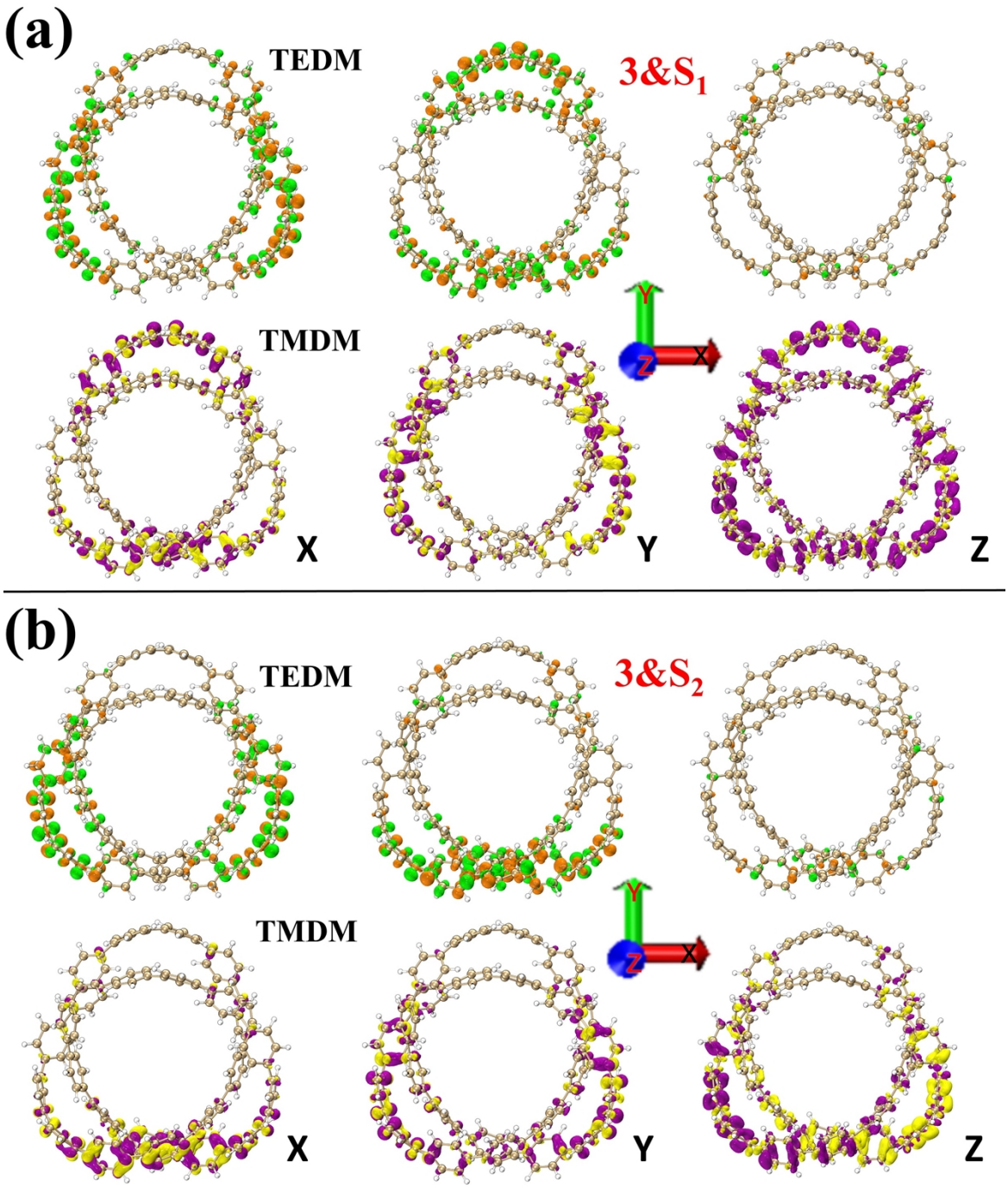

Figure S5. 3&S_1 (a), S_2 (b) are TEDMs\TMDMs in different directions. The green (orange) isosurfaces represents the positive (negative) transition electric dipole moment, and yellow (purple) isosurfaces represents the positive (negative) transition magnetic dipole moment.