Electronic Supplementary Information

Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives

Haitao Wang,[a,b] Fangyi Chen,[a] Xiaoshi Jia,[a] Huimin Liu,[a] Xia Ran,[c] Mahesh Kumar Ravva,[d] Fu-Quan Bai,[b] Songnan Qu,[e] Min Li,[*,a] Hong-Xing Zhang[*,b], Jean-Luc Brédas[*,d]

[a] Key Laboratory of Automobile Materials (MOE) &College of Materials Science and Engineering, Jilin University, Changchun 130012, China.

[b] Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, China.

[c] Department of Physics, School of Physics and Electronics, Henan University, Kaifeng, P. R. China

[d] Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology – KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia.

[e] Key Laboratory of Excited State Processes, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, Changchun 130033, China.

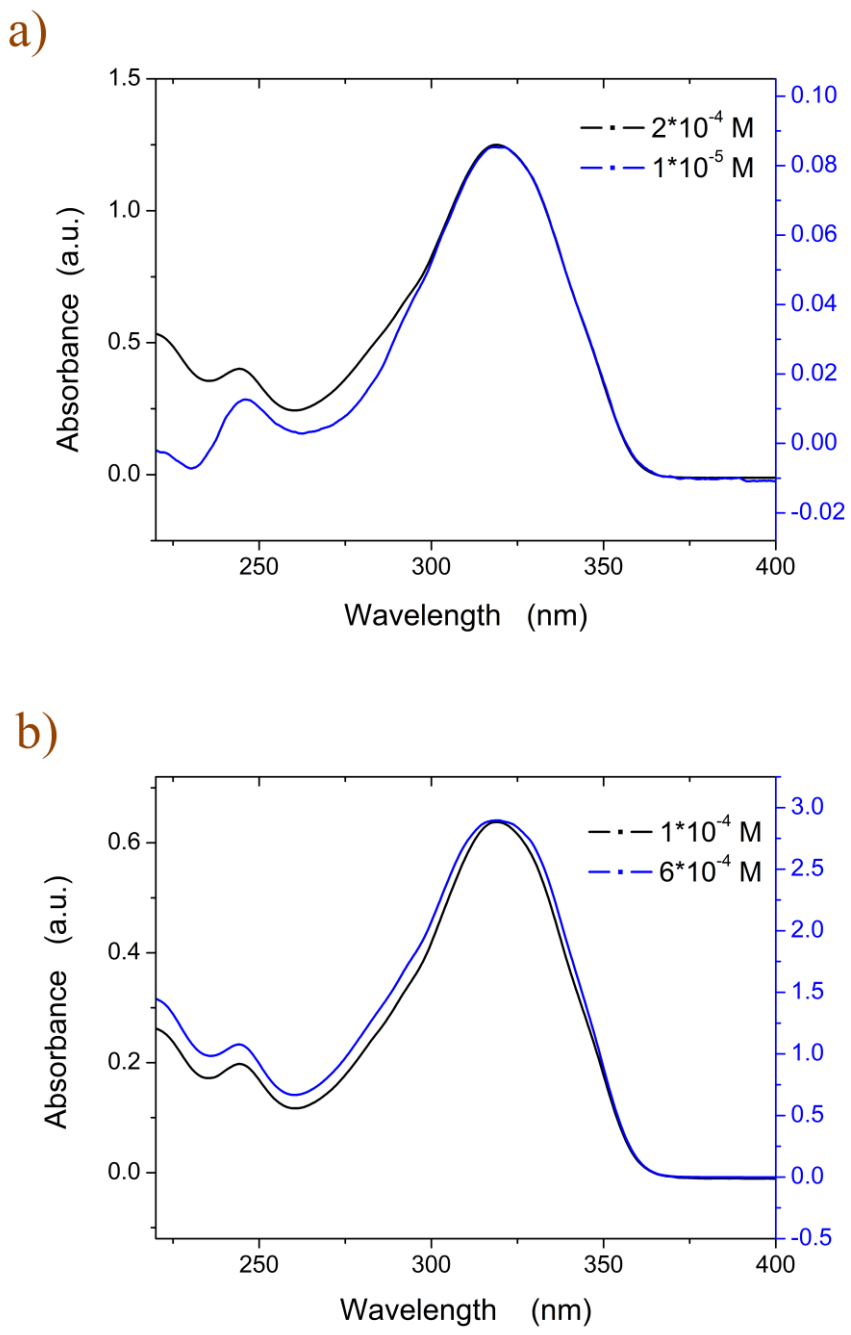

Figure S1 Comparing the UV-vis absorption spectra of BOXD-6 in tetrahedron at different concentrations.

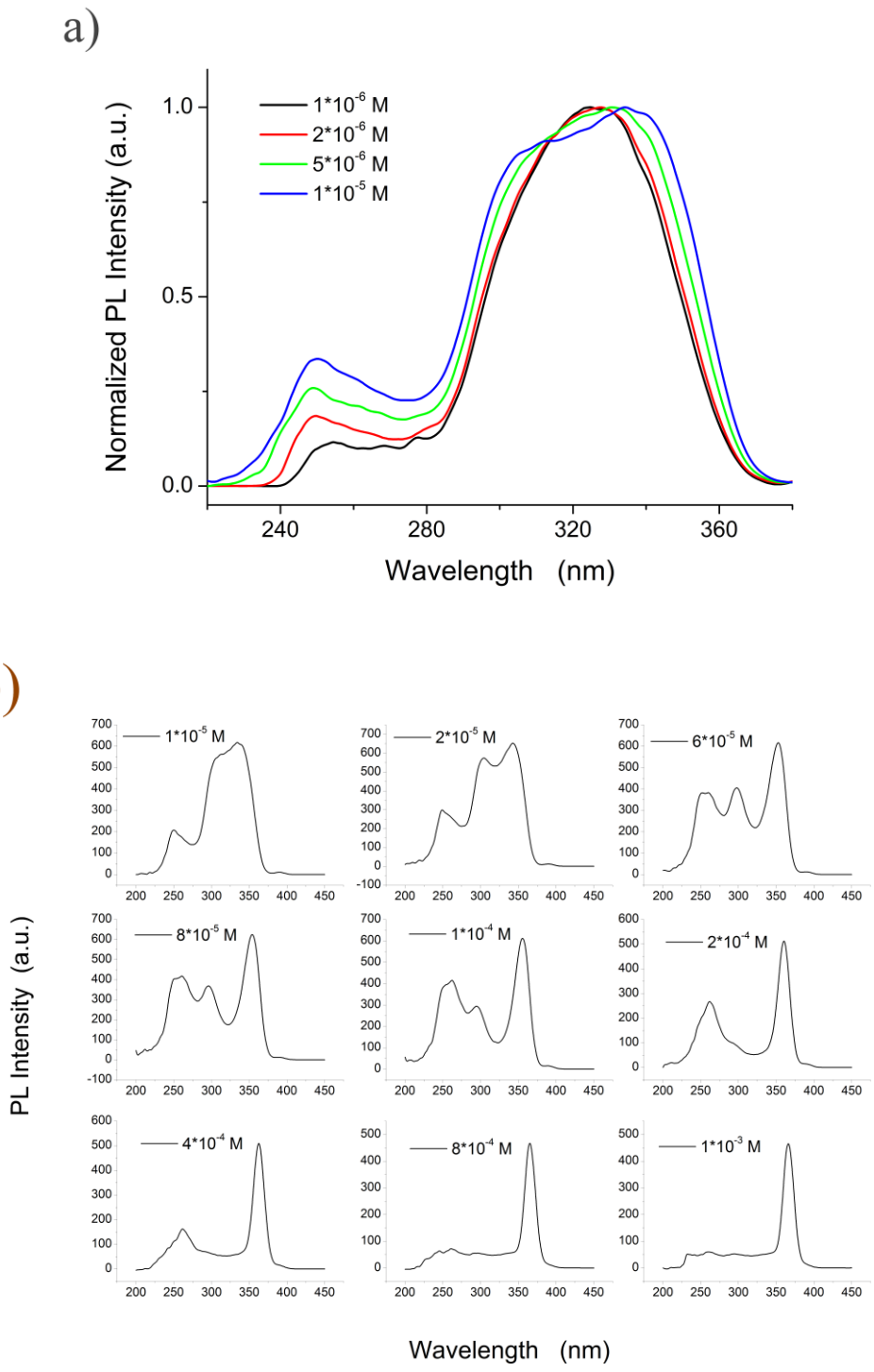

Figure S2 Excitation spectra of BOXD-6 in THF at different concentrations.

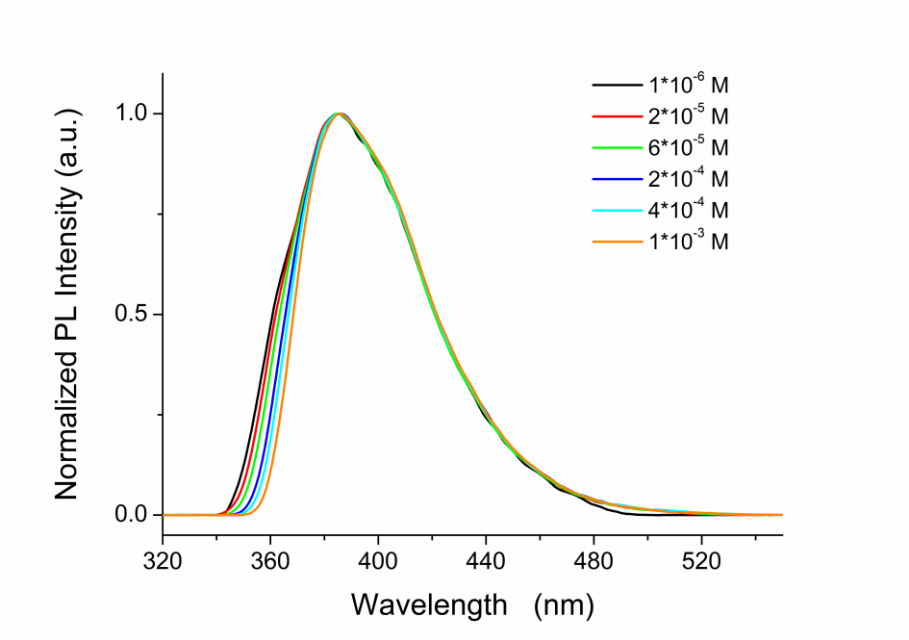

Figure S3 Normalized Photoluminescence emission spectra of BOXD-6 in THF at different concentration.

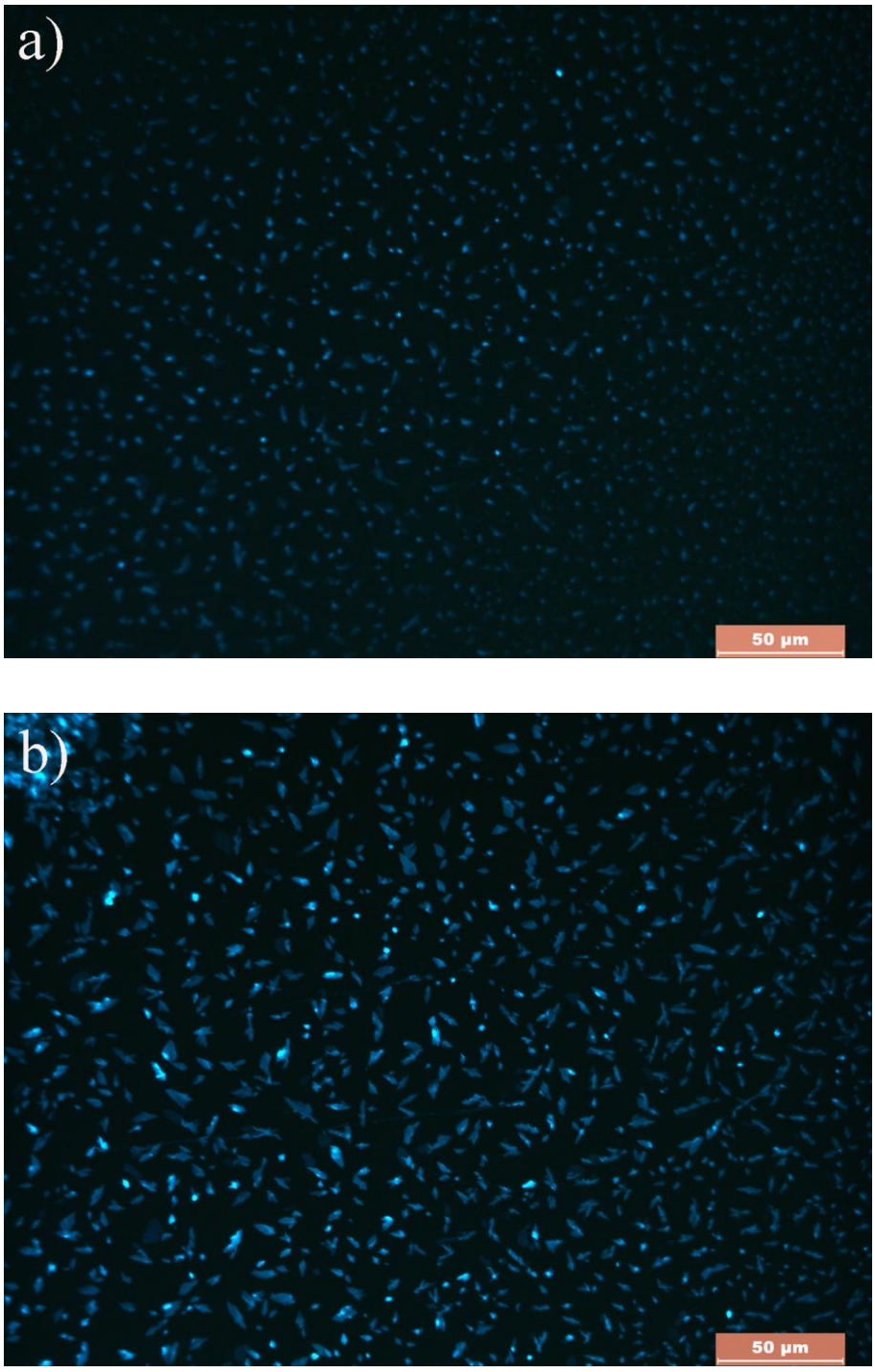

Figure S4 Fluorescence microscopic images of molecular aggregates of BOXD-6 from the THF solution at a) 1×10^{-4} M and b) 1×10^{-3} M.

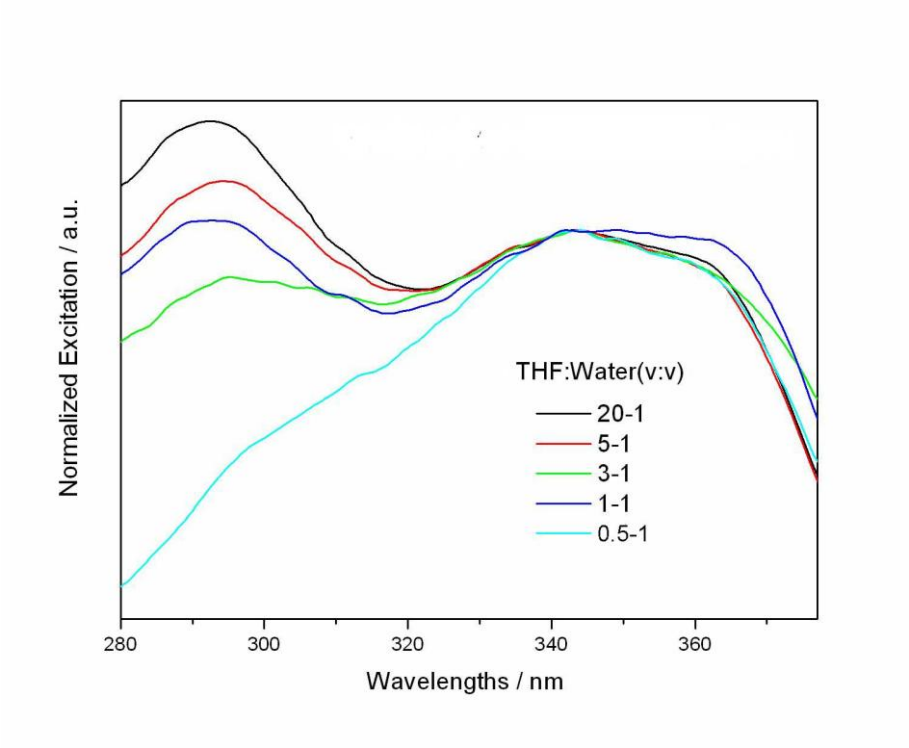

Figure S5 The effect of water ratio on excitation spectra of BOXD-6 in the precipitated particles by adding water into thick tetrahydrofuran solution.

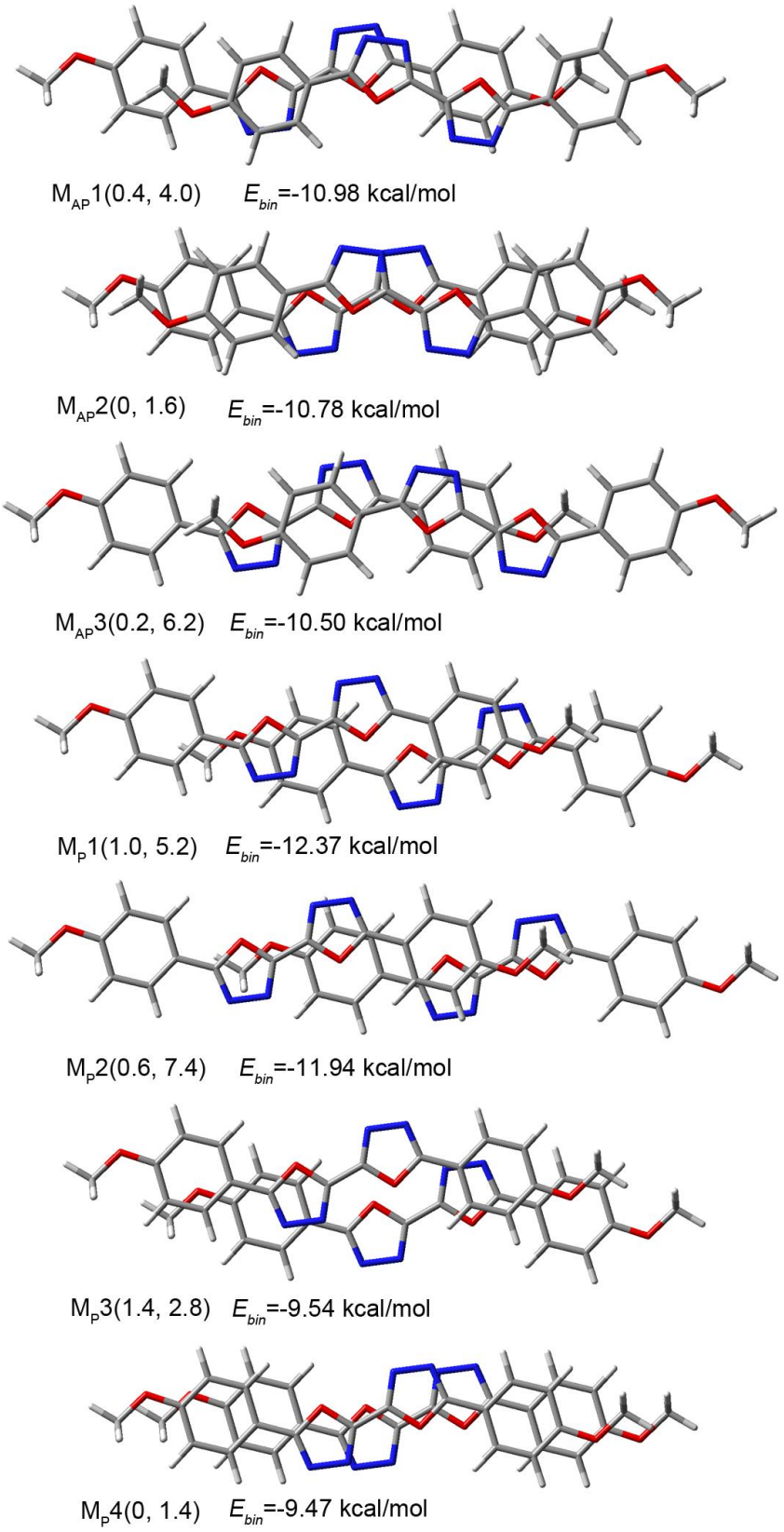

Figure S6 Energy-minimum molecular stacking structures of BOXD-1 found via PES scanning.

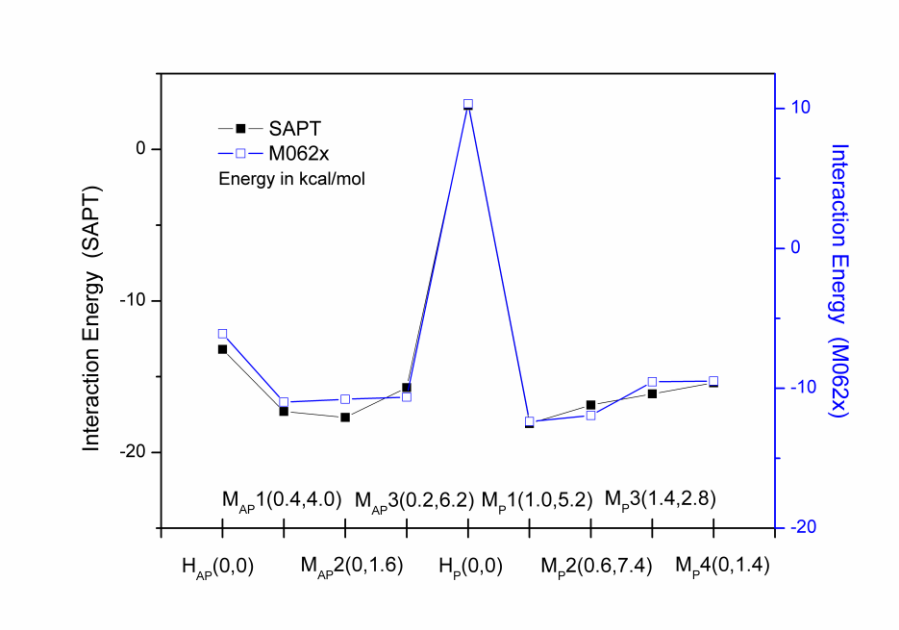

Figure S7 Calculated intermolecular interaction energy from an SAPT analysis and the M062x/6-31G** method.