

Supporting information for the article entitled

Systematic Investigation of Fluorescence Properties of Symmetric and Asymmetric Diazo[1,2-*a*:2',1'-*c*]quinoxaline Derivatives

Shoji Matsumoto*, Keisuke Sakamoto, and Motohiro Akazome

Department of Applied Chemistry and Biotechnology, Graduate School of Engineering, Chiba University, 1-33 Yayoicho, Inageku, Chiba 263-8522, Japan

E-mail address: smatsumo@faculty.chiba-u.jp

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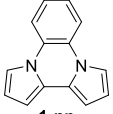

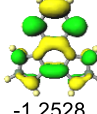
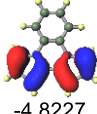
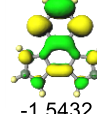
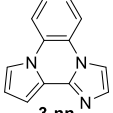
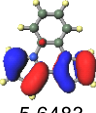
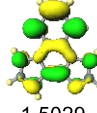

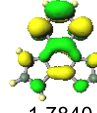
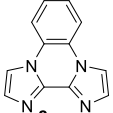
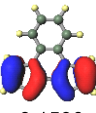
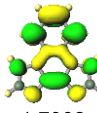
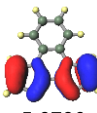
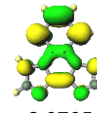
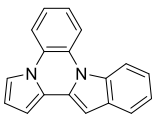
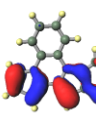
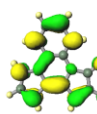
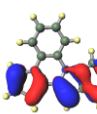
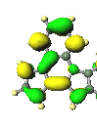
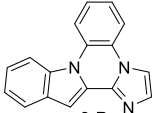
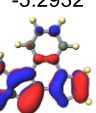
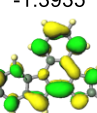
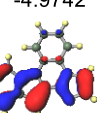
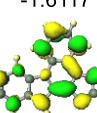
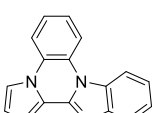
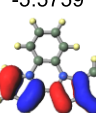
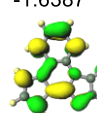
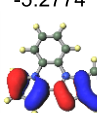
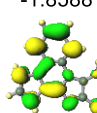
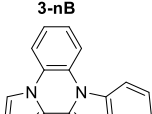
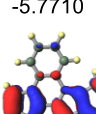
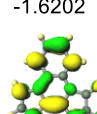
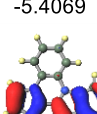
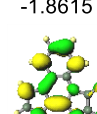
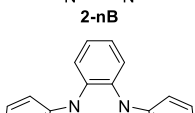
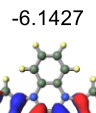
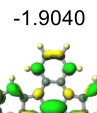
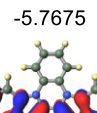
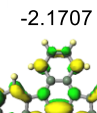
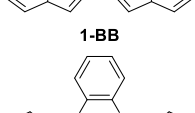
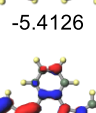
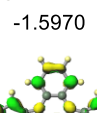
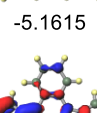
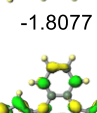
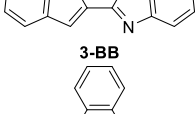
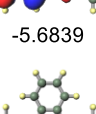
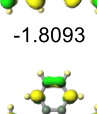
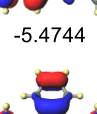
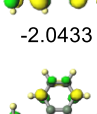
Compound	DFT		TDDFT	
	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
 1-nn	 -5.2224	 -1.2528	 -4.8227	 -1.5432
 3-nn	 -5.6483	 -1.5029	 -5.2344	 -1.7840
 2-nn	 -6.1590	 -1.7902	 -5.6730	 -2.0765
 1-nB	 -5.2932	 -1.3935	 -4.9742	 -1.6117
 3-Bn	 -5.5759	 -1.6387	 -5.2774	 -1.8588
 3-nB	 -5.7710	 -1.6202	 -5.4069	 -1.8615
 2-nB	 -6.1427	 -1.9040	 -5.7675	 -2.1707
 1-BB	 -5.4126	 -1.5970	 -5.1615	 -1.8077
 3-BB	 -5.6839	 -1.8093	 -5.4744	 -2.0433
 2-BB	 -6.2151	 -2.0645	 -6.0475	 -2.3530

Figure S1. The HOMO, LUMO, and their energies of all compounds discussed in the main text estimated by DFT and TDDFT (nstate=10) calculation after the structural optimization at the B3LYP/6-31+G level.

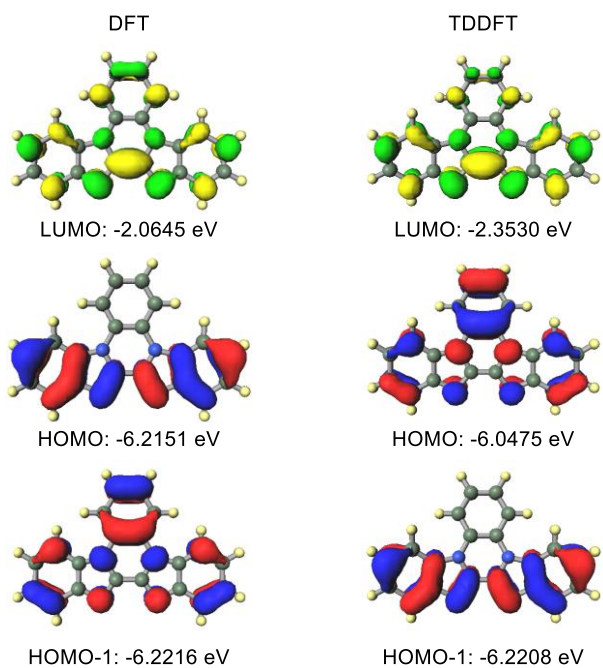


Figure S2. The orbitals and energies of **2-BB** estimated by DFT and TDDFT (nstate=10) calculation after the structural optimization at the B3LYP/6-31+G level.

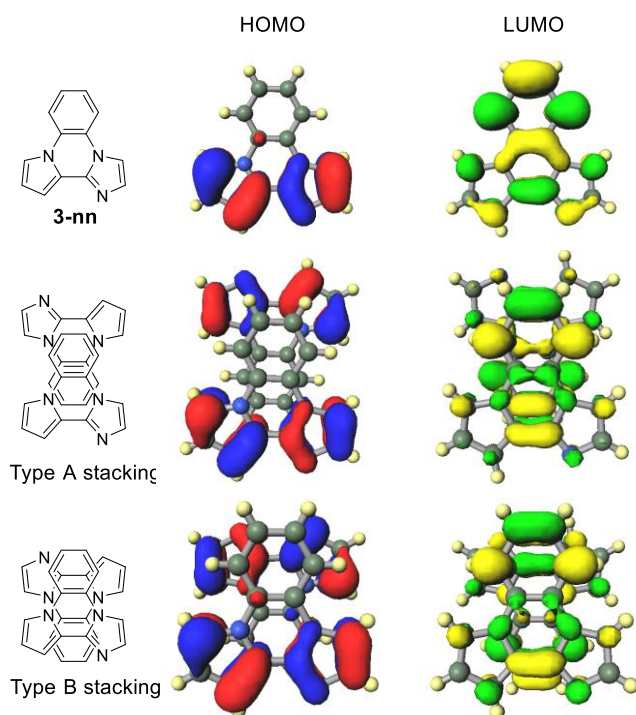


Figure S3. The HOMO and LUMO of **3-nn** for single molecule and each packing mode (type A and type B) by TDDFT calculation at the B3LYP/6-31+G level (nstate=10). The structures of type A and B stackings were obtained from single crystal X-ray analysis.

