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Structural Rigidity Accelerates Quantum Decoherence and Extends Carrier Lifetime in Porphyrin Nanoball: A Time Domain Atomistic Simulation

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Supplementary information

Table S1. Standard deviation of fluctuation of atoms of the porphyrin nanoballs.

Average atomic fluctuation (Å ³)	Zn	Cd
Т0	0.058	0.015
Т6	0.007	0.006
T14	0.003	0.003

Table S2. Comparison between the ground and excited state geometries of Zn-porphyrin nanoball (Zn-T0).

System	Ground state		Excited state	
	Major axis (Å)	Minor axis (Å)	Major axis(Å)	Minor axis (Å)
Zn-T0	50.890	24.780	50.893	24.781
	50.884	24.798	50.886	24.801

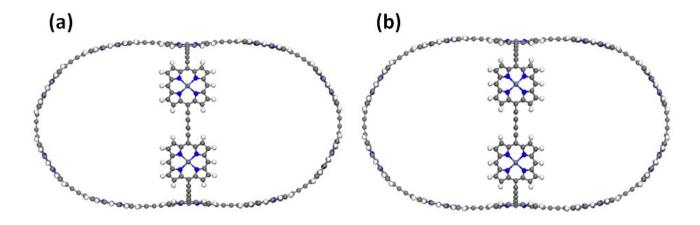


Figure S1: Ground (a) and excited state (b) geometries of Zn-T0 nanoball.