

Supplementary Files for:

## Bending a Photonic Wire into a Ring

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### 1. File overview

#### DFT and PM3 optimised geometries

Geometry file (.xyz) of the ***l*-P2·L** complex.

Geometry file (.xyz) of the ***c*-P24b·(T12)<sub>2</sub>** complex (PM3 level).

Geometry files (.xyz) of porphyrin nanorings (***c*-P12**, ***c*-P24**, ***c*-P12b**, and ***c*-P24b**) and linear oligomers (***l*-P4**, ***l*-P5**, ***l*-P4b<sub>3e</sub>**, and ***l*-P5b<sub>4e</sub>**) used for strain calculations.

#### MM optimised geometries

Geometry files (.xyz) of linear and curved conformations of ***l*-P24** used for strain calculations.

Geometry files (.xyz) of both classes of porphyrin nanorings ***c*-PN** and ***c*-PNb** from  $N = 9$  to 32, as well as linear oligomers (***l*-P4**, ***l*-P5**, ***l*-P4b<sub>3e</sub>**, and ***l*-P5b<sub>4e</sub>**) used for strain calculations.

#### Molecular dynamics simulations

Geometry (.xyz), trajectory (.gro), and topology (.top) files of ***c*-P24b**, ***c*-P24b·(T12)<sub>2</sub>**, ***c*-P24b·T12**, ***l*-P12e·T12a**, ***l*-P24·(T12)<sub>2</sub>** in binding modes A and B, and ***l*-P24·T12**.

Molecular dynamics parameters (.mdp) files for energy minimization, molecular dynamics production, NPT and NVT equilibrations.

## 2. File details

### Optimised geometries (DFT, PM3 and MM level)

All the DFT optimisations were performed using Gaussian 16/A.03<sup>1</sup> at PBE0+GD3BJ/Def2SVP level of theory.<sup>2,3</sup> PM3 optimisations were performed using MOPAC.<sup>4</sup> MM optimisations were carried out in GROMACS (v. 2019.2) with a double precision installation.<sup>5</sup> Structures were minimised using the steepest descent algorithm with a step size of 0.01 nm, a convergence threshold of 1 kJ mol<sup>-1</sup> and a maximum number of steps of 50000. Minimisation was done in vacuum with no periodic boundary condition and no cut-off for non-bonded interactions.

### Molecular dynamic simulations

All molecular dynamics (MD) simulations were performed in an isothermal-isobaric (NPT) ensemble at 300 K and 1 bar with a time step of 2 fs using GROMACS (v. 2019.2).<sup>5</sup> Simulations employed the General AMBER force field<sup>6</sup> with modifications to parameters for zinc ions and porphyrin connections as described above. Systems were minimised using the steepest descent algorithm for 5000 steps or until the maximum force on any atom was below 1000 kJ mol<sup>-1</sup> nm<sup>-1</sup> and subsequently equilibrated using a velocity-rescaling thermostat<sup>7</sup> and Parrinello-Rahman barostat.<sup>8</sup> All simulations were performed in explicit chloroform<sup>9</sup> with three-dimensional periodic boundary conditions. The box sizes were chosen by leaving 1 nm distance between solute and box boundary. Long-range electrostatic interactions were calculated using the particle mesh Ewald method.<sup>10</sup> All bond lengths involving hydrogen atoms were constrained with the LINCS algorithm.<sup>11</sup> All MD simulations were performed with the complete molecule including 3,5-bis(octyloxy)phenyl solubilising groups.

## 3. References

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