Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

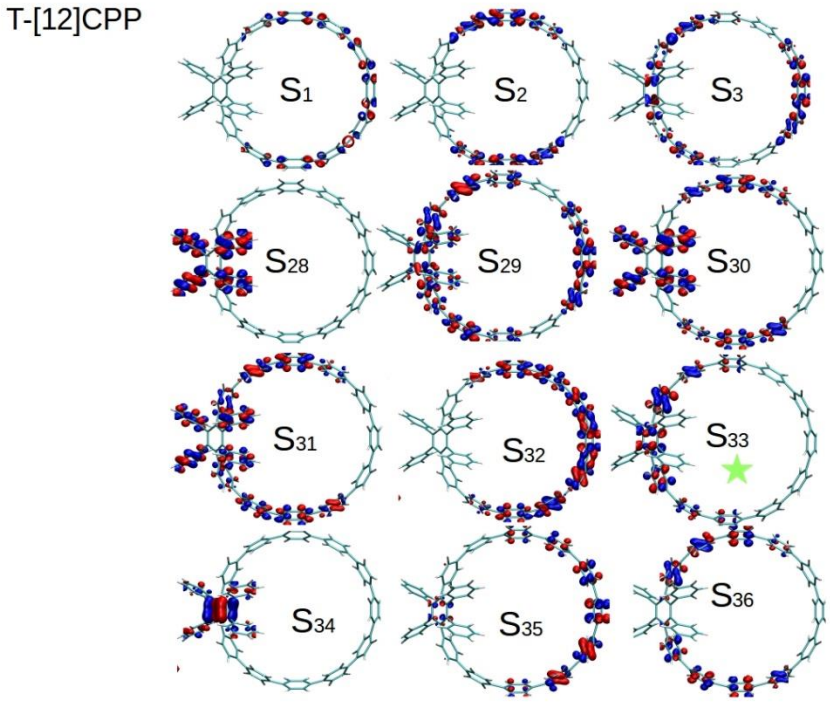
Supplementary information

Exciton-vibrational dynamics induces efficient self-trapping in a substituted nanoring

Laura Alfonso Hernandez[1], Victor M. Freixas[1], Beatriz Rodriguez-Hernandez[1], Sergei Tretiak[2], Sebastian Fernandez-Alberti[1*]and Nicolas Oldani[1]

[1]Departamento de Ciencia yTecnologia, Universidad Nacional de Quilmes/CONICET,B1876BXD Bernal, Argentina
[2]Theoretical Division and Center forIntegratedNanotechnologies, Los AlamosNationalLaboratory,Los Alamos, New Mexico 87545, USA

*corresponding author: sfalberti@gmail.com



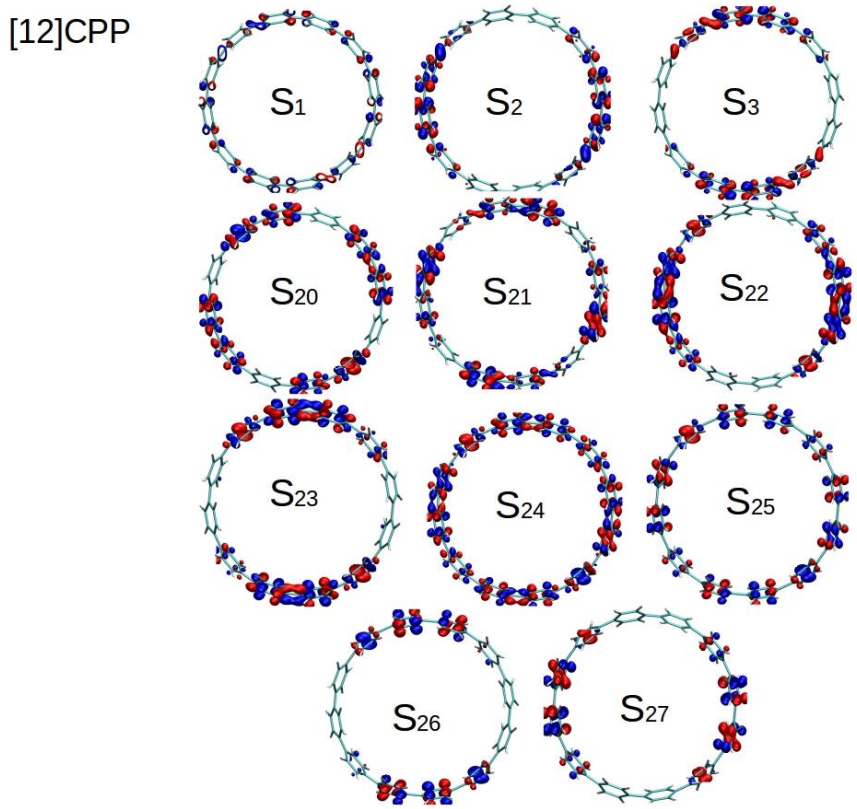


Figure S1. Spatial localization of the electronic transition densities for selected excited states of [12]CPP and T-[12]CPP-

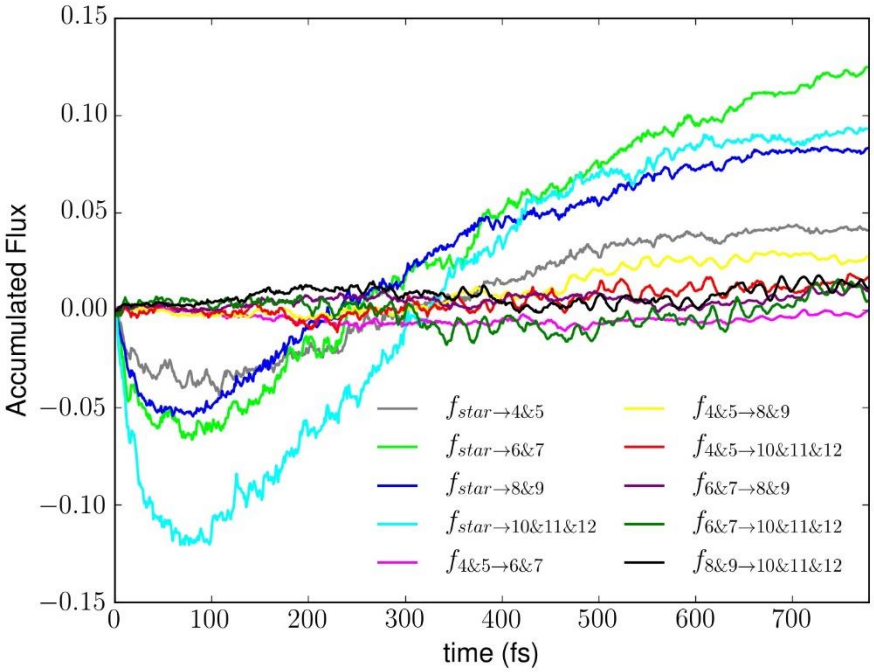


Figure S2. Accumulated fluxes among different ensembles of phenylene units during NEXMD simulations of T-[12]CPP. Units are numbered according to the pattern shown in Fig. 1(a)