Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Optical Control of Conjugated Oligomer Planarity SERGEI TRETIAK, Los Alamos National Laboratory, JENNY CLARK, Cavendish Laboratory, University of Cambridge, GUGLIELMO LANZANI , Lanzani — Using a sequential photo-excitation mechanism we observe the ultrafast conformational planarization of a large fluorene oligomer at $\sim$ 60fs timescale. Novel non-adiabatic excited state molecular dynamics (NA-ESMD) framework incorporating quantum transitions has been used to rationalize this phenomenon. Simulation show the ultrafast relaxation of the photoexcited wavepacket toward the lowest electronic excited state along the torsional coordinate. The process effectively 'locks' the oligomer into a planar state within 100 fs, with excess energy being dissipated into other vibrational modes. Ultrafast control of molecular conformation, as demonstrated here, could have impacts for molecular conformational switches for memory or molecular electronics.

Sergei Tretiak
Los Alamos National Laboratory

Date submitted: 27 Nov 2010 Electronic form version 1.4