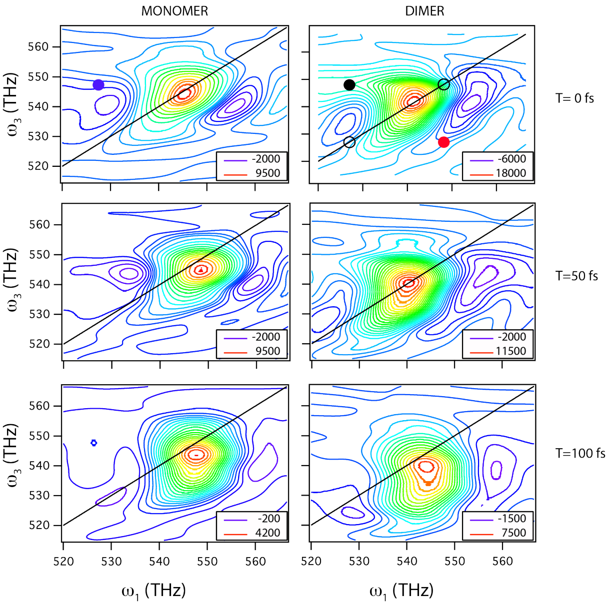
D2.3.1 Optical addressing of concatenated molecular logic machines: application to simple design systems

WP2, M12

Lead beneficiary: P3, UNIPD

As preliminary analysis, we studied by means of 2DES a simple dimer system (D) in which two quadrupolar A-π-D-π-A branching units (M) are connected by a C3 propyl chain [E.Collini et al., ChemComm, submitted]. The idea was to identify possible patterns of energy transfer to be included in concatenated machines logical schemes. 2D spectra at early times confirmed the presence of excitonic interactions in D, manifested by the presence of an upper cross peak, absent in the spectra of the monomer. This peak can be attributed to an ultrafast energy sharing between the two moieties in the dimer, which can be indeed related, from the logical point of view, to concatenation. However, more complex structures will be necessary to be really able to implement concatenation.

It should also be mentioned that the signal as a function of delay time showed oscillations, to of them present only upon dimerization. These two frequencies could be attributed to vibronic coherences, produced by the strong interaction between vibrational modes and excitonic transitions upon dimerization. This represents a further degree of complexity of the information included in 2DES which can be exploited for multivariate (also concatenated) logic schemes.



Experimental real 2D spectra of the monomer M (left panels) and corresponding dimeric species D (right panels) at population times *T=0,* 50, 100 fs. The filled dots indicate the cross peak positions.