D1.2.1 Principles of parallel computation and use of observables.
M12, WP1
Lead Beneficiary P2 (RDL-HUJI)

The partners of **WP1**, **P1** and **P2** designed molecular decision trees. This work(1) received considerable attention. A commentary was written on it in the same issue of PNAS where it appeared (2) and a summary was written for the website phys.org.(3) A decision tree provides the value of a logic function of several logic variables for all the possible combination of inputs. It can be viewed as a graphical representation of the truth table of a function, see Figure below. We designed molecular implementations in which all the outputs corresponding to all the inputs of multi variable Boolean and non Boolean functions are computed in parallel. The design relies on the fact that each time the system interacts with a perturbation, there is a change in time of the observables that is intrinsically parallel: all the observables of the system respond in parallel to the perturbation. The output is a function of the observables and different paths connect in parallel the initial state of the system to the read out. Since the interaction between the system and the perturbation is bilinear, one can implement parallel bilinear classical logical operations. The advantage of computing with observables is that there are N^2-1 matrix elements of the density matrix of a system with N states which completely characterize its time evolution, while there are only N occupation numbers. The scheme is scalable. The number of physical interactions with the perturbation determines the number of logic variables and the number of transitions between states at each interaction the maximum radix for the logic variable. The physical realization is based on the 2D photo echo spectroscopy implemented in **WP2** and was designed in collaboration with **P3**. In this set up, there are three-photon interactions with a bichromophoric molecule for which there are four accessible states which leads to 15 observables. Each time a photon interacts with the bichromophoric system, four different paths are possible, which leads to quaternary logic or in a simplified version to Boolean logic. We demonstrate the mode of operation of the machine using Lie algebra to describe the light-matter interaction. An example for a three variable Boolean function is given in the Figure below. An extension to electrical addressing using the set-ups realized in **WP3** is currently under investigation.

1. Fresch B, Hiluf D, Collini E, Levine RD, & Remacle F (2013) Molecular decision trees realized by ultrafast electronic spectroscopy *Proceedings of the National Academy of Sciences* 110:17183-17188.
2. Scholes G (2013) Light-powered molecular logic goes nonlinear *Proceedings of the National Academy of Sciences* 110:17167-17168.
3. Dambrot S (2013) The lightness of being: Smaller computer logic components through photon-molecule interaction. (phys.org, http://phys.org/news/2013-10-smaller-logic-components-photon-molecule-interaction.html).

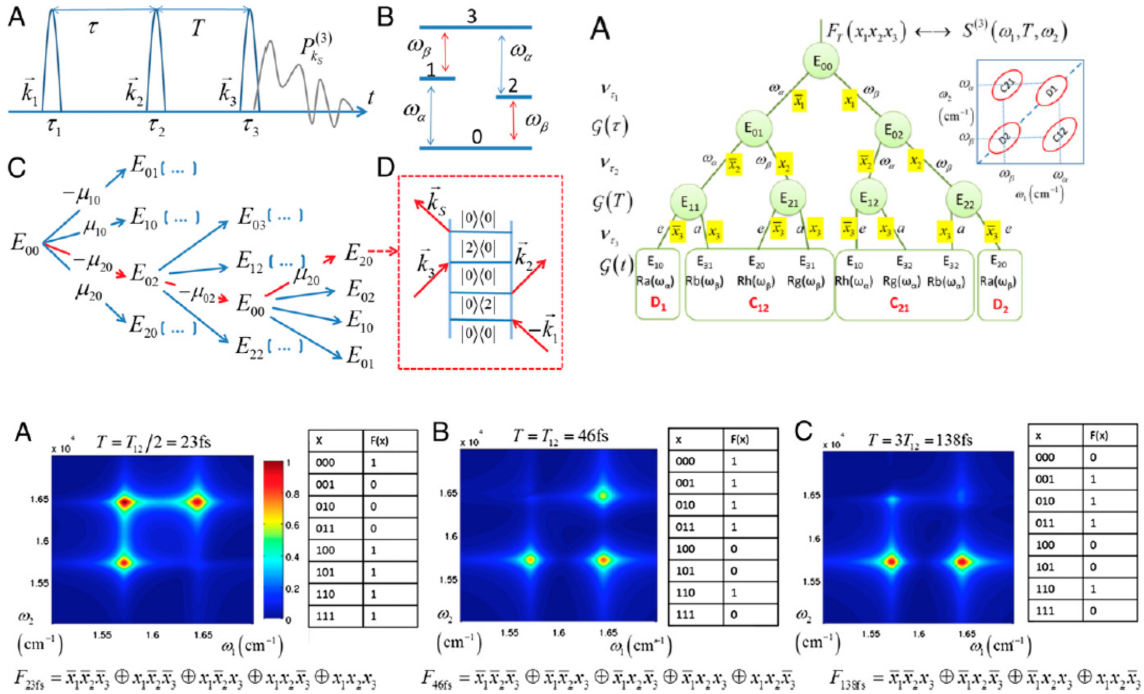

Figure 1. Scheme of the implementation of a molecular tree using 2D photoecho spectroscopy. Top Left : A : Time ordering of the 3 pulses sequence of the experimental set-up. B. Scheme of the level structure of the heterodimer in the exciton basis. C. The commutator tree describing the light-matter interaction at third order. D. A particular Feynmann path in the commutator tree (marked in red in C). Top right : The three level decision tree for a 3 variable Boolean function that can be implemented on the heterodimer for 3 light-matter interactions. The inset sows the the position of the peaks in the 2D map. Bottom. Examples of 3 Boolean functions of 3 variables that can be evaluated from the 2D map obtained by 2D photo echo spectroscopy of a heterodimer.