Molecular wires confined in zeolite L channels for an effective transport of electronic excitation energy: a synchrotron structural study

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Sunlight is the fundamental energy source sustaining life on Earth. Green plants are provided of very sophisticated and highly efficient tools to exploit light, they are able to harvest sunlight and to transport electronic excitation energy by means of a particular "antenna system" to reaction centers (natural photosynthesis).The development of an artificial system able to mimic the natural phenomenon has been a long-standing challenge. Artificial antenna systems can be realized once several organized chromophores are able to absorb the incident light and to channel the excitation energy to a common acceptor component [1-3]. The optical properties of the systems depend on the molecular packing inside the channels. Artificial antenna can be built by incorporating suitable guests into the one-dimensional channels of zeolite L (ZL). In this work we present a detailed structural study of two hybrid systems in which dyes (fluorenone and thionine) are encapsulated in zeolite L channels. These two molecules were chosen since it has been demonstrated that a "two –dyes antenna system" - in which fluorenone (FL) (donor molecule) and thionine (Th) (acceptor molecule) are organized in Zeolite L porosities - shows remarkable optical properties. Due to the impossibility of studying, from the structural point of view a "two –dyes systems", two "one-dye" hybrids (ZL/fluorenone and ZL/thionine) were firstly synthesized and characterized [4].

The results of thermogravimetric, IR, and X-ray structural refinements carried out for the one-dye ZL/FL and ZL/Th systems established that 1.5 molecules of FL and 0.3 molecules of Th per unit cell is the maximum loading, respectively. The FL carbonyl group strong interacts with a K^+ of the ZL. On the other hand, short distances between the carbon, sulfur and nitrogen atoms of Th and two water molecule sites, in turn at bond distance from the oxygen atoms of the main channel, suggested a water-mediated Th-ZL interactions. The energy transfer from excited FL molecules, forming the non-covalent nano-ladder in the ZL channel, and Th, deposited on the external surface of ZL particles, is currently under investigation.

In conclusion concerning the optical properties of our composites, no evidence of Davydov splitting emerged from our study, indicating that one of the main competitors of the FRET mechanism is not operative notwithstanding the close packed arrangement of FL. We believe that this feature is of overwhelming relevance in view of application of such a system in artificial antenna devices.

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