

**s9.m1.o3 Molecular Packing and Photoluminescence Efficiency in Thiophene-Based Oligomers.**

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The rational design of new organic molecular materials for application in electronics and photonics requires extensive investigation on the way they self-assemble in the solid state, since charge transport and light emission properties are strictly dependent on molecules collective behaviour. Single crystal X-ray structure analysis furnishes straightforward information on molecules supramolecular organization. Dissecting the elements governing the crystal packing gives information about the forces presiding over the organization of the same molecules in the thin films used for fabricating the electrical and optical devices and allows to establish a correlation between molecular structure and solid-state electrical and optical properties. Conventional thiophene oligomers display solid-state photoluminescence efficiencies on the order of only a few percent, owing to their packing modalities which cause strong intermolecular interactions leading to the dominance of radiationless pathways in the process of excitation decay. We will show that appropriate functionalization - in particular the transformation of one thienyl ring into the corresponding thienyl-S,S-dioxide - may dramatically change the molecular packing characteristics and lead to photoluminescence efficiencies which are more than one order of magnitude higher than those of conventional thiophene oligomers.

**s9.m1.o4 Methyl and ammonia rotation in molecular crystals.** P. Schiebel, *Institut für Kristallographie, Universität Tübingen, Charlottenstr.33, 72070 Tübingen, Germany*.

Keywords: neutron diffraction, dynamical disorder, hydrogen.

Bragg diffraction allows us to image the space-time average of the scattering density distribution in a crystal. In the case of neutron diffraction this distribution is given by the probability density function of finding a particular nucleus at a given position, multiplied by the coherent neutron scattering length  $b$  of that nucleus. If dynamic processes are present, neutron diffraction yields a direct long-time exposure of the dynamics. Due to the opposite signs of the neutron scattering lengths of protons and deuterons ( $b_H = -3.7$  fm,  $b_D = 6.67$  fm), protons, in contrast to deuterons, give a negative contribution to the nuclear scattering density.

In crystals, small molecules or molecular groups like  $\text{CH}_3$  and  $\text{NH}_3$  may show dynamical disorder and undergo one dimensional rotations around their 3-fold axis. For a free uniaxially rotor the protons have equal occupational probability at any position on a circle defined by the rotational radius. The corresponding density is homogeneously distributed on a ring. Any deviation from free rotation shows up in a deformation of the circle and/or in a modulation of the density on the circle. Therefore the observed density, obtained after a precise structure determination, serves as a basis for the development of more sophisticated models of the molecular dynamic. A model for the coupling of rotational and translational motion is given<sup>1-3</sup>.

At low temperatures the observed density has to be interpreted in a quantumstatistical treatment<sup>2,4</sup>. The solution of Schrödinger's equation gives the energy eigenvalues and the corresponding wave functions, from which the density is constructed, whereas the differences of the energy eigenvalues are directly observable with inelastic neutron scattering. Thus it is possible to interpret the nuclear density distribution, which is obtained by neutron diffraction at low temperatures and the energyspectrum, which is observed in inelastic neutron scattering, consistently by one dynamical model.

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