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Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude, Raum C10.013

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EPR Study of charge transfer co-crystals Structure/Function Relationship

Organic charge-transfer (CT) co-crystals exhibit unique electronic and magnetic properties depending on their molecular packing, structures and aggregated states which make them attractive materials for electronic devices.

Dibenzotetrathiafulvalene (DBTTF)/2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) co-crystal presents a segregated stacked packing, with a unitary degree of charge transfer. EPR temperature studies revealed that upon charge transfer the electron migrate through the stack from 18.6 Å at 5 K up to 19.42 Å at 300 K.

Co-crystals of Anthracene/ tetracyanoquinodimethane (TCNQ) have a mixed stacked packing, resulting in a localized spin with a unique long relaxation times. Here we present the results of our charge transfer co-crystals screening study, which resulted with four charge transfer co-crystals having mixed stack packing and long spin relaxation times: Tetramethylphenylenediamine (TMPD)/ tetracyanoquinodimethane (TCNQ), Naphthalene/ 1,2,4,5-Tetracyanobenzene (TCNB) and perylene/2,2'-Benzo[1,2-b:4,5-b']dithiophene-4,8-diylidene-bis-propanedinitrile (DTTCNQ).

In this study we were able to determine the criteria for charge transfer co-crystals with long spin relaxation times. In addition, EPR study upon photoexcitation of Anthracene/TCNQ co-crystals showed the formation of spin polarized radical-pair spectrum. Its EPR phase pattern indicates it is a triplet born radical pair.

