

etc. We are looking in particular for supramolecular organization in mixed crystals that can modify centrosymmetric structure of pure material into acentric structure of host-guest compound. Such approach can help to alter organization of strongly polarized donor-acceptor molecules in crystals and make them useful for applications as optoelectronic materials. In the mixed crystals of I and II organic components are benzene derivatives such as isomers of nitrotoluene, low-melting or liquid at room temperature. Crystal growth of these materials has been done using zone melting technique and molecular structure of these materials in pure compounds was compared with their structures in mixed crystals. It was found that number of acentric crystals in the series mixed crystals of I with nitrobenzene derivatives is higher than statistical expectation. Explanation of this phenomenon can be found in specific intermolecular interactions forming supramolecular associates in these materials.

Keywords: co-crystals, organometallic, Lewis acids

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#### Crucible rotation dependence of oxygen concentration during solidification of multicrystalline Si

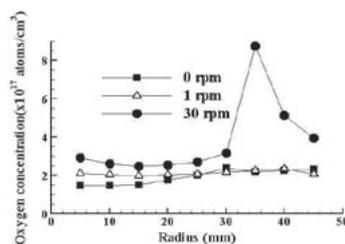
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Multicrystalline silicon (mc-Si) has a market share of more than 50 % in all photovoltaic materials. Oxygen in mc-Si forms defects, which decrease conversion efficiency of solar cells. Therefore, control of oxygen concentration in a silicon ingot is an important issue to improve conversion efficiency. A crucible is rotated during solidification process to control and/or homogenize oxygen concentration. Since oxygen concentration is affected by a melt flow. The radial flow velocity is suppressed by the crucible rotation because centrifugal force acts in the opposite direction [1]. From view of this point, we optimized crucible rotation during solidification process in order to minimize oxygen concentration in the growth direction and homogenize that in the radial direction. Fig. 1 shows oxygen concentration as a function of radius in the ingot measured by FTIR at 50 mm from bottom of the ingot. Oxygen concentration at crucible rotation rates of 0 and 1 rpm is homogenized in the radial direction. Therefore, we concluded that crucible rotation rate from 0 to 1 rpm is optimal rotation rate.

References

[1] K. Kakimoto, et al., *Int. J. Heat Mass Transfer*, 35 (1992) 2551.



Keywords: multicrystalline silicon, crystal growth, FTIR

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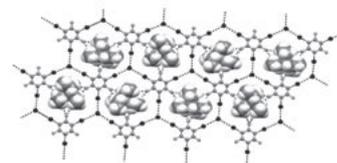
#### Supramolecular anion coordination networks with (6.3) cation-templated topologies

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In this presentation we show the use of the halogen bonding between various naked iodide anions and 1,3,5-trifluoro-2,4,6-triiodobenzene (TFTIB) for the deliberate construction of anionic honeycomb-like networks with a degree of precision and accuracy that is unusual for crystal engineering. The 3-fold symmetry of TFTIB elicits the three coordinate profile of I<sup>-</sup> thanks to a mutual induced fitting process of the valencies of interacting partners. Anionic networks characterize all the complexes obtained, where cations sit in the hexagonal cavities, filling the potential voids and stabilizing these 2D networks. TFTIB functions as a reliable tridentate and trigonal tecton in halogen bonding-based crystal engineering [1].

[1] Metrangolo P., Meyer F., Pilati T., Resnati G., Terraneo, G., *Chem. Commun.* 2008, 1635-1637.



Keywords: halogen bonding, anion coordination, supramolecular chemistry

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#### Co-crystallisation and crystal engineering

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As pharmaceutical interest in co-crystals continues to grow, understanding why and how certain molecular functionalities aid or inhibit the formation of co-crystals has become paramount. In this paper we looked at the use of crystal structure database searching and molecular modeling in order to develop protocols for designing co-crystals of commercial compounds that contain different molecular functionalities. Searching the Cambridge Structural Database for known co-crystals containing the desired intermolecular interactions helped identify the class of compound most likely to form co-crystals with our compounds of interest. Using binary and ternary phase diagram data co-crystallisation of a known compound with various formers were carried out from melt, solution and solid phases. The solid phases obtained were subsequently characterized using single crystal x-ray diffraction and to a lesser extent powder diffraction and DSC. Molecular modeling, using Materials Studio, of all the systems studied was used in order to try and understand the success/failure of specific systems in forming co-crystals. In general it was found that those systems which formed co-crystals, the heterodimer present in the co-crystal structure was more energetically favourable than the two homodimers.

Keywords: co-crystallisation, ternary phase diagrams, crystal engineering