

## MS41-04 | SUBSTRATE INDUCED POLYMORPHISM OF ORGANIC ELECTRONIC MOLECULES

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Crystallisation of molecular crystals at defined substrate surfaces can lead to unknown polymorph phases. Several examples are known for organic electronic molecules, but also for pharmaceutical molecules. These polymorphs can have considerably different optical, electronic, mechanical and dissolution properties which influences their potential applications. A first step of understanding the origin of substrate induced phases is the determination of the molecular packing. A combination of grazing incidence x-ray diffraction with molecular dynamics simulation is used for crystal structure solution. Recently, also single crystal diffraction is used for crystal structure solution of substrate induced phases. We selected a number of different molecules and demonstrate fundamental properties of the crystalline structure in relation to the bulk crystal structure. It is shown that confirmation of the molecular packing with the substrate surface is an important parameter, additionally the different polymorphs can show fundamental different packing motifs like herringbone packing and stacking of aromatic rings. In a subsequent step the importance of the crystal growth kinetics is presented which causes the substrate induced polymorph and finally the thermodynamic stability of these phases. The selected examples are molecules which forms van der Waals crystals like pentacene, oligothiophenes, benzothieno-benzthiophene based molecules but also examples from molecules with hydrogen bonds are discussed like dibromo-indigo and phenytoin.