

## Self-assembly monolayer of PbPc: a starting point for substrate induced polymorphism

Polymorphism, which represents a phenomenon that a solid material could crystallize into different structures. Those structures are then described as polymorphs of the corresponding substance. Practically, most crystallizations occur on substrates, where the substrate acts as a catalyst for the crystallization process. Apart from the catalyzing, substrates induce a more special effect on the crystallization: the formation of substrate-induced polymorph (SIP), which means the formation of new polymorphs that exist only in the vicinity of the substrate and that differ from the bulk phase.

Another line of research, although conceptually connected to substrate-induced phases, is the self-assembly of molecules physisorbed on highly-regular surfaces (2D crystallization). This 2D crystallization has been studied intensively in recent years to achieve: e.g. tune of surface properties, desire molecular pattern on surface.

My research aims to marry the substrate-induced polymorphism and 2D crystallization for organic molecules. The SAM is assumed as a bridging layer between substrate and SIPs and considered to affect the following crystal growth. Currently, lead phthalocyanine (PbPc) is used as the target molecule and highly orientated pyrolytic graphite (HOPG) as substrate. Multiscale computational chemistry approaches have been applied to study the SAM of PbPc. Combined with high resolution scanning-probe techniques, structural and energetic properties of this monolayer have been investigated both experimentally and theoretically.

