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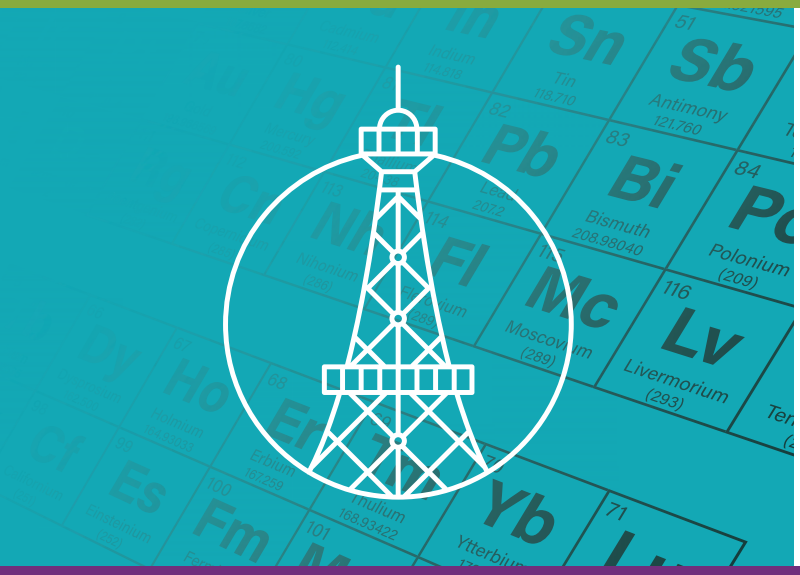
ABSTRACT BOOK



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CL100

MODELLING CRYSTAL POLYMORPHS AND RELATED PHASE TRANSITIONS IN SEMICONDUCTING POLYMERS: POLY(3-ALKYLTHIOPHENES)

1. Materials for Energy by Computational Design

#CL100

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Abstract

Applications of materials are strongly dependent on solid-state organization both at the molecular scale and at the dimensions of crystallites. The ways materials, and more specifically polymers, respond organizing or reorganizing in different crystalline polymorphs due to changes in temperature, pressure or other physical variables, are hence of fundamental interest. Semiconducting polymers are particularly challenging because they normally organize poorly in the solid state and, investigating their phase transitions, even devising sensible initial and final models has proven difficult, largely because of disorder. [1] This depends on the ambivalent features of their molecular structure characterized by a π-conjugated main chain, essential for charge transport, and relatively long alkyl side chains allowing facile processing of such materials.

The presentation will concentrate on poly(3-alkylthiophenes) (P3ATs), widely used p-type semiconductors in organic electronics, in energy harvesting and in storage devices. P3AT's are a relatively simple but highly representative family of conjugated polymers, extensively studied for decades both experimentally and theoretically. [1] Atomistic molecular dynamics (MD) simulations of observed transitions of various P3ATs from the stable and relatively ordered, but rare form II polymorph[2], to more common form I modifications can be followed continuously, under appropriate circumstances[3]. This study has been made possible by the development of force-fields adapted for P3ATs [4], and by the identification of selected reliable starting models [2]. The molecular assemblies resulting from the simulation process display substantial reorganization, characterized by the development of defects of various kind, in part frozen in upon cooling the models. Significant new insights, both with respect to structure development and to the merits of the adopted computational methodologies [5] will be discussed, attempting to access models of increasing reliability also for the form I polymorph family of P3ATs.

References

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