

PARIS, FRANCE 2019

50th
GENERAL
ASSEMBLY

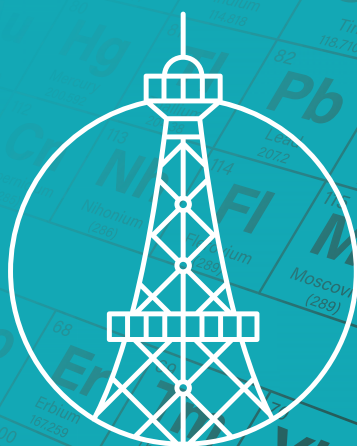
(5-12 July, Palais des Congrès, Paris)

&

47th
IUPAC WORLD
CHEMISTRY
CONGRESS

(7-12 July, Palais des Congrès, Paris)

ABSTRACT BOOK



IUPAC

IUPAC CENTENARY CELEBRATION

www.iupac2019.org

TABLE OF CONTENTS

› PLENARY LECTURES	3
› CHEMISTRY FOR LIFE / Invited speakers	11
› CHEMISTRY FOR LIFE / Oral communications	53
› CHEMISTRY FOR LIFE / Poster communications	199
› CHEMISTRY FOR ENERGY AND RESOURCES / Invited speakers	877
› CHEMISTRY FOR ENERGY AND RESOURCES / Oral communications	944
› CHEMISTRY FOR ENERGY AND RESOURCES / Poster communications	1 143
› CHEMISTRY FOR THE ENVIRONMENT / Invited speakers	1 445
› CHEMISTRY FOR THE ENVIRONMENT / Oral communications	1 514
› CHEMISTRY FOR THE ENVIRONMENT / Poster communications	1 699
› CHEMISTRY AND SOCIETY / Invited speakers	2 240
› CHEMISTRY AND SOCIETY / Oral communications	2 251
› CHEMISTRY AND SOCIETY / Poster communications	2 270
› CHEMISTRY EDUCATION / Invited speakers	2 282
› CHEMISTRY EDUCATION / Oral communications	2 295
› CHEMISTRY EDUCATION / Poster communications	2 327
› IUPAC AND CHEMISTRY: A CENTURY OF HISTORY / Invited speakers	2 439
› IUPAC AND CHEMISTRY: A CENTURY OF HISTORY / Oral communications	2 452
› IUPAC AND CHEMISTRY: A CENTURY OF HISTORY / Poster communications	2 470
› YOUNG SCIENTISTS PROGRAMME / Invited speakers	2 477
› SPECIAL SYMPOSIA / Invited speakers	2 495
› SPECIAL SYMPOSIA / Oral communications	2 524
› SPECIAL SYMPOSIA / Poster communications	2 570
› CHEMISTRY ACROSS THE THEMES / Invited speakers	2 584
› CHEMISTRY ACROSS THE THEMES / Oral communications	2 661
› CHEMISTRY ACROSS THE THEMES / Poster communications	2 941
› VARIOUS TOPICS / Poster communications	3 408



1. Materials for Energy by Computational Design

#CL100

M. Casalegno ¹, G. Raos ¹, A. Famulari ¹, T. Nicolini ¹, S.V. Meille ^{1*}

Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano - Milano (Italy)

*Corresponding author(s).

Email: stefanovaldo.meille@polimi.it (S.V. Meille)

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

- [1] J. Rivnay, S. C. B. Mannsfeld, et al, Chem. Rev., 112, 5488 (2012).
- [2] A. Buono, H.S. Nguyen et al, Macromolecules, 43, 6772 (2010).
- [3] M. Casalegno, T. Nicolini, A. Famulari, G. Raos, R. Po, S.V. Meille, Phys.Chem.Chem.Phys.,20, 28984 (2018).
- [4] M. Moreno, M. Casalegno, et al, J. Phys. Chem. B 114, 1591 (2010).
- [5] A. Famulari, G. Raos et al, J. Phys. Chem. B, 116, 14504 (2012).