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A7-THU-AM3-2 - Computational microscopy of conducting polymer PEDOT:PSS (poly(3,4-ethylenedioxythiophene:polystyrene sulfonate)

A7. Materials for Organic Electronics

Igor Zozoulenko[1] , *Mohsen Modarresi*[1, 2], *Aleksandar Mehandzhiyski*[1], *Juan Felipe Franco-Gonzalez*[1, 3]

[1] Laboratory of Organic Electronics, Linköping University, Sweden

[2] Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran

[3] Autonomous University of Madrid, Medicine Campus, Lab-3, Madrid, Spain

Introduction/Purpose

The Poly(3,4-ethylenedioxythiophene) polymerized in the presence of polystyrene sulfonate (PEDOT:PSS) is one of the most technologically important conducting polymers for organic electronics. A massive amount of experimental studies has been devoted to investigation of various aspects of morphology of PEDOT:PSS. At the same time, a theoretical understanding of its complex morphology and corresponding simulation and modelling are practically missing.

Methods

In the present paper we report computational microscopy study based on the Martini coarse grained Molecular Dynamics (MD) simulations of PEDOT:PSS focussing of the formation of the granular structure, PEDOT crystallites, and the effect of pH on the material morphology.

Results

PEDOT:PSS morphology is shown to be sensitive to the initial distribution of PEDOT and PSS in the solution, and the results of the modelling suggest that the experimentally observed granular structure of PEDOT:PSS can be only obtained if PEDOT/PSS solution is in the dispersive state on the initial crystallization stages. The variation of the pH is demonstrated to strongly affect the morphology of PEDOT:PSS films altering their structure between granular-type and homogeneous one. It also affects the size of crystallites and the relative arrangement of PEDOT and PSS chains. It is shown that the crystallites in PEDOT:PSS are smaller than those in PEDOT with molecular counterions such as PEDOT:Tosylate, which is consistent with available experimental data.

Conclusions

The predicted changes of PEDOT:PSS morphology with variation of pH can be tested experimentally, and the calculated atomistic picture of PEDOT:PSS films (not accessible by conventional experimental techniques) is instrumental for understanding of the material structure and building realistic models of PEDOT: PSS morphology.

Selected references

Mohsen Modarresi, Juan Felipe Franco-Gonzalez,and Igor Zozoulenko,*Computational Microscopy Study of Granular Structure and pH Dependence of PEDOT:PSS*. Physical Chemistry Chemical Physics, 2019 accepted