Session 3 Session Notes

From Modelling to Experimental Characterisation for Energy Materials

Introduction

The session aims to correlate computer modelling and experimental characterisation, in application to the increasingly important area of energy materials. Two thematic sub-areas are first addressed: solar cells and batteries, and applications of both physics-based and data-based modelling approaches are considered. Discussion will be directed so as to identify key research problems relevant to the modelling of solar cells, taking into account characterisation data for organic semiconductor materials. Further, industrial problems relevant to the modelling of Li-ion batteries will be discussed, as exemplified by the modelling-based detection of material defects in graphene anodes or separators.

Following the impulse talks, broader discussions and collaborations within the EMMC are envisaged to follow. Expertise in multi-scale multi-physics modelling of energy materials is specifically solicited as well as joint efforts for the development of Open Platform tools and examples, for teaching and public communications on the subject. Collaborations are also sought with the sister society, EMCC, facilitating a MODA of each modelling example to be linked to its corresponding CHADA and characterisation results.

Objectives

The main objective of this session is to encourage new efforts of the EMMC community towards the modelling of energy materials. Specific collaborations are sought in:

- multi-scale multi-physics modelling of energy materials,
- data-based modelling of energy storage materials and devices,
- Open Platform modelling tools and examples for energy materials, for education purposes,
- Linking & Coupling Computational Chemistry to Electromagnetics (proposed Task Group),
- Linking MODAs and modelling results to CHADAs and characterisation results.

Chair

Malgorzata Celuch (QWED, PL)

Impulse 1

Ferry Kienberger (Keysight Research Labs, AT)

Development of Li-ion battery models from electro-impedance spectroscopy data

Impulse 2

Olivier Douheret (MateriaNova, BE)

Application of modelling tools for the electrical characterisation of organic semiconductors

Impulse 3

Georg Gramse (Johannes Kepler University, AT)

Joint Application of EM FEM and Data-based Modelling for Detection of Small Defect Structures in Batteries

Impulse 4

Marzena Olszewska-Placha (QWED, PL)

Modelling of energy materials and electrical test-fixtures: developments and Open Platform implementation linking MODAs and CHADAs

Background information and documents

This session is anchored within the "Model Development" Focus Area of the EMMC.

Sun, S.-S., Dalton, L. R. Introduction to Organic Electronic and Optoelectronic Materials and Devices. 2nd Edition, CRC 2019. ISBN 9780367868086

Coropceanu, V., Cornil, da Silva Filho, D. A., Olivier, Y. Silbey, R., Brédas, J. -L., Charge Transport in Organic Semiconductors, Chem. Rev. 2007, 107, 926−952, https://doi.org/10.1021/cr050140x

Lampert, M. A., Mark, P. Current Injection in Solids, Academic Press, Inc., New York, and London, 1970

Moerman D., Sebaihi, N., Kaviyil, S. A., Leclère, Ph., Lazzaroni, R., Douhéret, O., Towards a unified description of the charge transport mechanisms in conductive atomic force microscopy studies of semiconducting polymers, Nanoscale, 2014, 6, 10596-10603, https://doi.org/10.1039/C4NR02577F

Desbief, S., Hergué, N. Douhéret, O., Surin, M., Geerts, Y., Dubois, Ph., Lazzaroni R., Leclère, Ph., Nanoscale investigation of the electrical properties in semiconductor polymer - carbon nanotube hybrid materials, Nanoscale, 2012, 4 (8), 2705-2712. https://doi.org/10.1039/C2NR11888B

Celuch, M., Douhéret, O., Korpas, P., Michnowski, R., Olszewska-Placha, M., Rudnicki, J., "Portable low-cost measurement setup for 2D imaging of organic semiconductors", IEEE MTT-S Intl. Microwave Symp.2020, LA, 21-26 June 2020, https://doi.org/10.1109/IMS30576.2020.9224053

Douhéret, O. Théron, D. and Moerman, D., "Exploring the Capabilities of Scanning Microwave Microscopy to Characterize Semiconducting Polymers", MDPI, Applied Science, 2020, 10(22), 8234, https://doi.org/10.3390/app10228234

Nawfal Al-Zubaidi R-Smith, Georg Gramse, Manuel Moertelmaier, Manuel Kasper, Ferry Kienberger. Advanced Self-Discharge Measurements of Lithium-Ion Cells and Comparison to Modeling. 2020 IEEE International Instrumentation and Measurement Technology Conference (I2MTC), (2020).

Nawfal R-Smith, Mike Leitner, Ivan Alic, David Toth, Manuel Kasper, Ferry Kienberger, Andreas Ebner, Georg Gramse. Assessment of Lithium Ion Batteries aging by combined Impedance Spectroscopy, Functional Microscopy and Finite Element Modelling, in preparation.

www.qwed.eu/quickwave.html

M. Celuch and M. Olszewska-Placha, "QuickWave conformal FDTD modelling: electromagnetics and beyond", EMMC-CSA Workshop on Industrial Impact of Materials Modelling, Turin 8-10 July 2019, https://www.qwed.eu/publications/EMMC_Turin2019_poster.pdf

M. Olszewska-Placha, M.Celuch, T. Le Quang, A. Gungor, J. Hoffmann, J. Smajic, J. Rudnicki, "Open access CAD, EM tools, and examples for teaching microwaves", Proc. 23rd Intl. Conference on Microwaves, Radar and Wireless Communications MIKON-2020, Warsaw, 5-8 October 2020, https://www.qwed.eu/publications/MIKON_Warsaw2020_accepted_1.pdf

M.Celuch, M. Olszewska-Placha, J. Rudnicki, A. Gungor , J. Smajic, and J. Leuthold, "Open platform GUI for comparative FDTD and FEM computation of material microwave measurement scenarios", Proc. 19th Biennial IEEE Conference on Elecromagnetic Field Computation CEFC 2020, 16-19 November 2020, https://www.qwed.eu/publications/CEFC_Pisa2020_accepted.pdf

NanoBat Open Platform Tools and Examples: https://www.qwed.eu/nanobat.html

Discussion points and questions

The following questions summarise the issues for this session.

- In what respects are energy materials *different*? To what extent the existing EMMC competencies are applicable?
- Does characterisation data sufficiently substitute for the missing knowledge of the physics of energy materials? Can data-based modelling foster further developments in the physics?
- Is it feasible to perform multi-physics modelling, coupling computational chemistry to electromagnetics?
- Are our modelling efforts compatible with the needs of industry, in the fields of energy storage and harvesting?
- Can we increase popularity Open Modelling platforms? Will they compete with commercial software?
- Is it feasible to try and link every MODA to a corresponding CHADA? Will the twinning of modelling and characterisation data increase the trust in both?
- How to increase public awareness of modelling for energy storage? Could modelling act as a saving mechanism to foster development of energy storage?