Subarea POB3.6: Modeling and investigation of physicochemical properties of materials

Title of the presentation: Design of functional materials based structures for applications in electronics, optoelectronics and gas sensors

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Abstract:

The progress of the science in the last decades allowed the fabrication of materials films with thicknesses of nanometers. Such films in (opto)electronic devices (i.e. transistors, solar cells, gas sensors or biosensors) are often combined into multi-layered heterostructures of materials with different properties. The effectiveness of a device is determined by properties of component layers. The key issue are processes occurring on the surface and interface between materials or between a material and atmosphere. The most important for electronic devices effectiveness are electronic, chemical and morphological properties of materials. Thus, the prediction of those properties and physicochemical processes occurring at the interfaces are crucial for design of structures to be applied. In the era of high computational power, new possibilities have been opened in materials science. The properties of solid state can be predicted before the preparation of physical samples. Application of quantum chemistry modelling of studied materials can be used in the pre-selection of the most promising structures, limiting the experimental measurements to a narrow group of structures with optimal properties. Therefore, the cost and the time needed to characterize new structures are reduced and effectiveness of the research is improved.

The presented work shows the possibilities of the application of new methodology based on theoretical modelling prior experimental characterization for understanding the physicochemical processes on the surfaces and interfaces in the structures for applications in electronic devices. As an example, the modelling of sarin and sarin's simulant, dimethyl methylophosphonate (DMMP) interactions with metallo-phthalocyanines (MPcs), confirmed by experimental results is presented [1]. The outcome of this study provides crucial information for sarin sensor's design. Besides the results of sarin sensors modelling results, the wider possibilities of the new methodology application in design of structures for electronic devices are discussed.

Ref:

[1] H. Aldahhak, P. Powroźnik, P. Pander, W. Jakubik, F. B. Dias, W. G. Schmidt, U. Gerstmann, M. Krzywiecki, J. Phys. Chem. C 124 (2020) 6090–6102.