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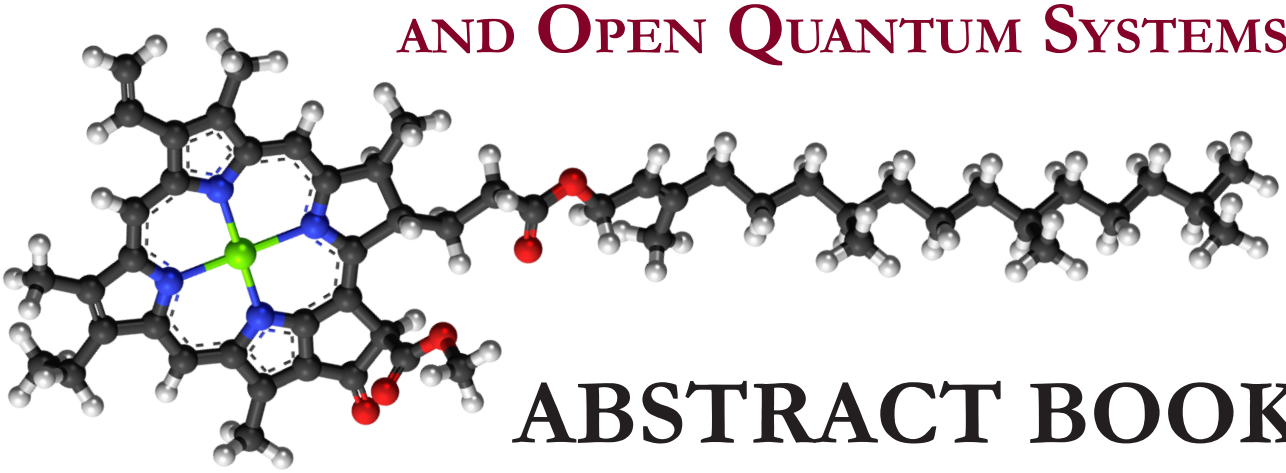

ABSTRACT BOOK

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MODELLING OF STRUCTURAL AND EXCITATION PROPERTIES OF NOVEL LIGHT-SENSITIVE ORGANIC COMPLEXES

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Light-sensitive molecular systems are extensively studied for both theoretical considerations (to gain insight into the physics behind light-activated processes) and practical reasons (possible applications include optoelectronics and nanoscale devices). New materials are constantly produced and presented for investigation which aims to aid in understanding and optimizing their properties. One group of such materials are photochromic compounds. Changes in absorption spectrum of these compounds during photoexcitation indicate energy transfer and structural transformations of the system, which are reversible (by thermal dissipation or by excitation of a different wavelength) in many cases. These compounds are proposed to be used as molecular switches and for high density data storage [1]. Another group of materials are molecular complexes containing heavy metal atom, such as Pt or Ir. Such complexes are regarded as one of the most promising materials for emitter layer of organic light-emitting diodes (OLEDs) because of their high efficiency and wavelength tunability [2]; research in this area is crucial in development of OLED devices.

A couple of recently synthesized organic complexes are presented – photochromic indolo[2,1-b][1,3]benzoxazine compound [3] and organic-metallic bis(2-phenylbenzothiazole)-iridium-acetylacetonate ((pbt)2Ir(acac)) molecular complex (Fig. 1) and its derivatives [4]. Spectroscopic measurements of the complexes are shortly discussed. Several computational methods for determining atomic structure and excitation properties of the compounds are described, and the results of the calculations using those methods are examined. While the evaluation of static properties (such as ground state structure and absorption spectrum of the molecule) has become computationally easier and more common today, modelling of dynamic parameters from first principles is still a challenging task. Some problems in this area and possible ways to resolve them are reviewed.

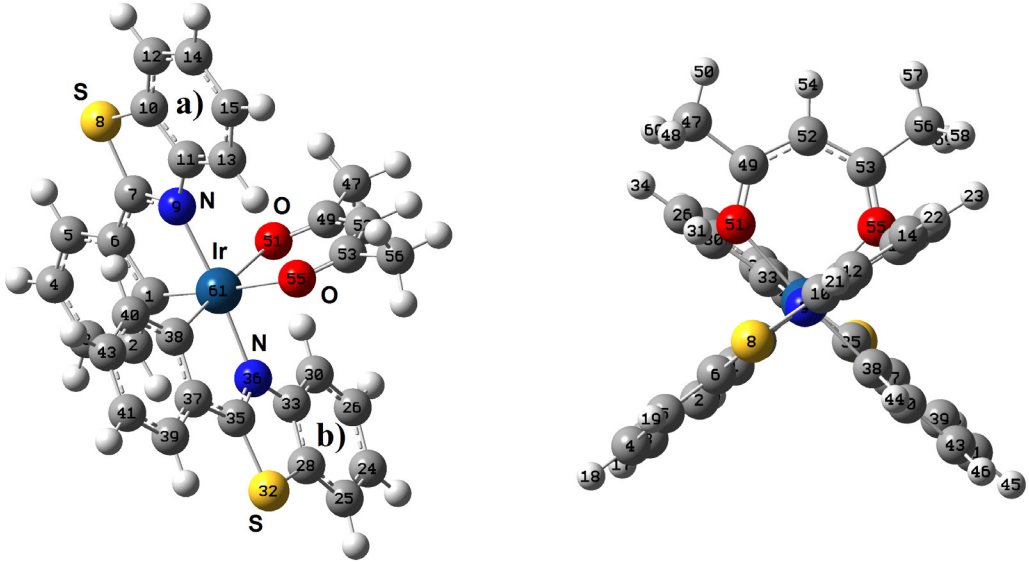

Figure 1. Molecular structure of phosphorescent $(pbt)_2Ir(acac)$ complex

[1] M. Irie, Chem. Rev., **100**, 1683 (2000)
[2] C. Jiang, W. Yang, J. Peng, Adv. Mater., **16**, 537 (2004)
[3] V. Amankavičienė, W. Holzer, S. J. Asadauskas, A. Šačkus, Intl. Conf. on Organic Synthesis, **58** (2006)
[4] S. Toliautas, J. Šulskus, K. Kazlauskas, S. Juršėnas, Intl. Conf. on Electronic Prop. of Organic Systems, **12** (2011)