

## Institute of Advanced Chemistry of Catalonia Seminars

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### ***Chemoinformatics analysis of high performance compounds for materials science and engineering***

**Date**

10:00 am  
September 16<sup>th</sup> 2019

**Location**

“Sala de Actos” room  
Institute of Advanced Chemistry of Catalonia (IQAC-CSIC)  
C/Jordi Girona 18-26, 08034 Barcelona

#### **Abstract**

Based on application of fragment approach in QSPR developed by Igor I. Baskin (Moscow State University) systematic analysis of chemical structure – property relationships for several groups of chemical compounds is provided:

Polymers: refraction, thermal stability, etc.

BODIPY dyes: absorption and emission properties.

Porphyrins: efficiency in DSSCs.

Liquid crystals: transition temperatures and classification.

Dyes for textile coloration: colour and colour fastness of water-soluble azo dyes on fibres of different nature.

The examples of collected databases and the results of their chemoinformatics analysis are discussed.

#### **Research**

1998-2000 Chief of the ISUCT group of researchers - INTAS-OPEN-97-487 in co-operation with Centro de Investigación y Desarrollo, belonging to the “Consejo Superior de Investigaciones Científicas” (Spain), Universidade da Beira Interior (Portugal), Institute of Bio-organic Chemistry of Russian Academy of Sciences.

Title of the project: Physicochemical study of liposome interaction with surface of fibrous material in textile dyeing.

2012-2017 Scholar of “Hundred Talents of Hubei”, chief of the project: Development of database and investigation of structure-property relationships for textile dyes, Hubei province, WTU, China

2019-date Participant of of the Russian Science Foundation project on synthesis. Research and application of BODIPY dyes