F I Ş A

raportului de activitate în anul 2023 pentru membrii titulari,
membrii corespondenți și membri desemnați ai Secțiilor de Științe ale AŞM

I.Titlul, numele şi prenumele, secţia de ştiinţe a AŞM

M. c. Ţucherblat Boris, **Secția de Științe Exacte și Inginerești**

II. Activitate ştiinţifică (participarea în proiecte de cercetare)

III.Activitatea în anul de referinţă (date statistice)

Articole în reviste cu factor de impact cu indicarea IF	6

IV. *Rezultate ştiinţifice obţinute în anul de referinţă (100-200 de cuvinte)*

1. Our research in 2023 have been focused on the problem of molecular quantum cellular automata (QCA) that promise fundamentally new principals of nano-electronics and computing with molecules. We have developed a vibronic theory of clocking in molecular QCA. The clocking mechanism is considered for a trigonal trimeric mixed-valence (MV) system with one mobile electron, which is shown to act as the dimeric unit encoding binary information (Boolean states **0** or **1**) coupled to the third redox center (**Null** state). The model includes electron transfer between the three centers, vibronic coupling of the mobile charge with the "breathing" modes and the two electric fields, one collinear to the dimeric unit, which controls the binary states, and the second one, perpendicular to this unit, performing clocking. In the framework of the adiabatic approximation the potential surface of the trimeric system has been studied and the condition determining switching and clocking have been analyzed in terms of the two controlling fields, as well as on the vibronic and the transfer parameters. A thorough understanding of the site populations is achieved through the quantum-mechanical solution of the vibronic problem maintaining the adiabatic condition for the controlling fields. It is shown that a MV trimer can act as a molecular clocked QCA cell, with favorable conditions being a positive electron transfer parameter and sufficiently strong vibronic coupling.
2. The effects of electronic and vibronic interactions on the specific heat release occurring in course of nonadiabatic switching of the electric field polarizing the one-electron mixed-valence dimer is analyzed within the framework of the vibronic model. The search for the optimal parametric regime from the point of view of minimizing heat release is carried out taking into account the requirement to maintain a strong nonlinear response of the dimer to the applied electric field. Calculations of the specific heat release and the response performed in the framework of the quantum mechanical vibronic approach show that although the heat release is minimal at weak electric field acting on the dimer in combination with weak vibronic coupling and/or strong electron transfer, while such combination of the parameters is incompatible with the requirement of a strong nonlinear response. Unlike this, for molecules exhibiting strong vibronic interaction and/or weak transfer, a rather strong nonlinear response can be obtained even with very weak electric field, which, in turn, ensures low heat release. Thus, we can conclude that an efficient strategy to improve characteristics of molecular quantum cellular automata devices or other molecular switchable devices based on mixed-valence dimers consists in usage of molecules subjected by the action of weak polarizing field, which are characterized by strong vibronic coupling and/or weak transfer.
3. This part of the work has been focused on the optical properties of the rare-earth ions in doped crystals. The rare-earth ions in crystals such as terbium ($YTaO4:Tb^{3+}$) and europium ($YTaO_4:Eu^{3+}$)-activated yttrium tantalate phosphors have a number of attractive features that predetermine their crucial role in practical application in contemporary optoelectronic devices. We employ the group-theoretical arguments aimed to reveal the group-theoretical classification of the crystal field levels and selection rules for the allowed optical transition between the crystal field components of Tb3+ and Eu3+ of the low symmetry crystal field in the activated yttrium tantalate phosphors. We also establish possible polarization rules for the lines corresponding to the allowed transitions. We deduce the symmetry-assisted results for the selection rules in the optical transitions accompanied by the absorption/emission of the vibrational quanta. The selection rules for the vibronic satellites of the zero-phonon lines are expected to be useful for the identification of the lines in the spectra of rare-earth ions with a weak vibronic coupling. The results of the low-temperature measurements of photoluminescence under the 325 nm excitation are in compliance with the group-theoretical analysis. The aim of the paper is to establish symmetry-assisted results that are the background of the quantitative crystal field theory based on the quantum-mechanical consideration. In this part of the work we report the luminescence properties of nanosized undoped and Eu2+ (1%) doped SrAl2O4 phosphors. Photo luminescence (PL) and cathodoluminescence (CL) analyses were applied to

characterize the phosphors. The qualitative energy level scheme of doped crystal SrAl2O4:Eu2+ and nature of defects in undoped phosphor is proposed and discussed. Within a simplified model of a single vibration and linear vibronic coupling the shape-function of the vibrationally assisted band (Pekarian) is analyzed with the emphasis on the vibrational structure. We propose an approximate approach to pass from the discrete Pekarian distribution to the structureless crystal field spectra taking into account phonon dispersion. This approach is expected to be useful for the description of the shape of the bands when the electronic levels are close to the conduction band of the host crystal.

V. Membru/președinte al comitetului organizatoric/științific, al comisiilor, consiliilor științifice de susținere a tezelor

Numele, prenumele	**Evenimentul (conferință, consiliu de susținere etc.)**	**Perioada**	**Calitatea (membru, președinte ș.a.)**
1,	25th International Symposium on the Jahn-Teller Effect	14th-18th May 2023	Member of the International Organzing Committee

Redactor / membru al colegiilor de redacţie al revistelor naţionale / internaţionale

Nr.	**Numele, prenumele**	**Revista**	**Calitatea (membru, redactor, referent)**
1.	Boris Tsukerblat	• ***Magnetochemistry*** *(*an international, reviewed journal). **Journal Rank:** JCR - Q2 (*Chemistry, Inorganic & Nuclear*) / CiteScore - Q2 (*Chemistry (miscellaneous)*), **Impact Factor:** 2.7 (2022);	*Member of the Editorial Board*

VI. ***Participări la foruri științifice:***

Manifestări științifice internaționale (în străinătate)

Nr	*Numele, prenumele, titlul ştiinţific participantului*	*Titlul manifestării organizatori/instituția organizatoare/țara*	*Perioada desfășurării evenimentului*	*Titlul comunicării/raportului susținut*
	Boris Tsukerblat, Shmuel Zilberg, Andrew Palii	North America-Greece-Cyprus Workshop on Paramagnetic Materials and the Current Trends in Molecular and Nanoscale Magnetism Conference, Spetses, Greece, May 8-12, 2023	May 8-12, 2023	In Quest of Controllable Electron Transfer Aimed to Performance Optimization of Molecular Quantum Cellular Automata Boris Tsukerblat, Shmuel Zilberg, Andrew Palii

Lista lucrărilor publicate în anul de referință (*conform Anexei 2***)**

Articole în reviste cu factor de impact WoS/ SCOPUS

1. M. Nazarov, D. Spassky, M.G. Brik, B. Tsukerblat, About the nature of luminescent bands in undoped and Eu^{2+} doped $SrAl_2O_4$ phosphors, Optical Materials 145, 114377 (2023).

2. A. Palii**,** V. Belonovich, S. Aldoshin, S. Zilberg, B. Tsukerblat, Mixed-Valence Bridged Norbornylogous Compounds as Switchable Cells for Molecular Quantum Cellular Automata: A Compromise between High Polarizability and Low Power Dissipation, The Journal of Physical Chemistry A 127 (43), 9030-9039 (2023).
3. A. Palii, D. Korchagin, K. Kondrina, S. Aldoshin, S. Zilberg, B. Tsukerblat, Spin polarization effects in trigonal mixed-valence complexes exhibiting double exchange supported by external spin-cores, *J. Chem. Phys.* 158, 194303 (2023)
4. A. Palii, V. Belonovich, B. Tsukerblat, In the quest for an optimal parametric regime of nonadiabatic switching ensuring low heat release in conjunction with high polarizability of mixed-valence molecular dimers, Phys. Chem. Chem. Phys. 25, 17526-17534 (2023).
5. S. Zilberg, B. Tsukerblat**,** A. Palii, Polaronic Mechanism of Vibronic Localization in Mixed-Valence Cation Radicals with a Non-Conjugated Chromophore on the Bridge, Phys. Chem. A 127, 15, 3281–3292 (2023).
6. M. Nazarov, B. Tsukerblat, Optical Lines in Europium and Terbium-Activated Yttrium Tantalate Phosphor: Combined Experimental and Group-Theoretical Analysis, Optics 4 (3), 510-524 (2023).

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Semnătura **Țucherblat Boris**