Project No. 02320 / Grant No. JPMXP0723833151

Report form of Joint Research Project at ZAIKEN (FY2023)

Title of Project	Study on the local structure around dilute dopants in optical materials		
Priority Area	III-B(Energy saving & Structures), III-C(Energy saving & Properties)		
Continuation of the project in FY2021 and FY2022			
Name of Main Applicant	Mikhail G. Brik		
Institution	Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia	**title**	Professor

Aim of the research project

The advanced optical materials have gained great attentions to realize sustainable societies. To get efficient optical materials, a doping technique is often employed. To understand their efficiency of light emission and absorption mechanisms, it is essential to know the geometric and electronic structures. In particular, local structure around dopants is of paramount importance for enhancement of the phosphors' brightness. The main aim of the proposed research is to understand the mechanisms of the emission enhancement of the Mn^{4+}-doped phosphors and photon up-conversion in the rare-earth ions doped materials. These topics are now extremely actively studied by many research groups worldwide, which is explained by numerous practical applications of these materials for solid state lighting, photovoltaics, agriculture etc. Despite high research activity in this field, the mechanisms underlying these phenomena have not yet been understood with strong experimental and theoretical evidences. In the present joint research with Prof. Yamamoto, we would like to focus on the experimental and theoretical studies of the Mn^{4+} -doped (and co-doped with other cations) phosphor materials and rare-earth ions doped oxide powders, which will include the X-ray diffraction, UV-Vis, photoluminescence, ESR measurements and theoretical density functional theory (DFT)-based calculations to understand the local structure effects on the optical properties.

Contents and results of the research

1. Several series of Mn^{4+} doped double perovskites (RE_2MgMO_6, *RE*=La, Y, *M*=Ti, Sn) were synthesized. Influence of chemical composition on the Mn^{4+}-emission spectra was studied. The samples were characterized by the X-ray diffraction (XRD) and optical spectroscopy methods.
2. The ABO_4 (*A*=Ca, Sr, Ba, *B*=Mo, W) samples doped with the Er^{3+} ions were synthesized and their upconversion properties were studied.
3. First-principles calculations of the Mn^{4+} energy levels in $CaMO_3$ (M=Ti, Zr, and Sn) were performed.
4. The hybrid organic-inorganic perovskite materials were synthesized and their photovoltaic properties were studied experimentally and by means of the first principles calculations.
5. Machine-learning methods were applied to identify correlations between the structural and electronic properties of garnets. In addition, the same methods were used to describe and predict emission energy of the red phosphors based on the Mn^{4+} and Cr^{3+} ions. These works are in progress now.
6. First-principles calculations of the structural, electronic, elastic properties of the Mn^{4+}- and Cr^{3+}-doped phosphor materials were continued. The most important parameters, such as the energy of the ^2E-$^4A_2$ emission transition and the crystal field strength were calculated. This is important for a deeper understanding of red phosphors performance, in particular, thermal quenching effects.
7. A visit to Prof. T. Yamamoto laboratory was arranged between March 10 and 20, 2024. Several meetings with Prof. T. Yamamoto group members were organized, where the students presented and discussed their recent results. Active discussions were held; the plans for publications of those results and for the future research were outlined. Prof. M.G. Brik presented a tutorial lecture "Transition metal ions for lighting and spectroscopy". The visit was very fruitful for the development of joint research plans. Two researchers from Tajikistan – Dr. Dilshod Nematov and Dr. Amondullo Burhonzoda – also participated in these meetings.
8. An online meeting for the joint research at ZAIKEN, Waseda University was held on March 1, 2024. Prof. M.G. Brik gave a presentation entitled "Cr^{3+} and Mn^{4+} ions for optical thermometry and lighting".
9. Active cooperation with the research groups from the USA, Poland, China and Tajikistan was strengthened further during this project implementation.
10. Comparing the initial plan of our activities with the summary of the obtained results, we conclude that the expected objectives of the project were achieved.

Outputs of the project (publications, presentations, patents)

An invited talk: "Influence of local environment of emission center ions on the luminescence property of phosphor materials" by Prof. Tomoyuki Yamamoto was presented at the EMRS Fall Meeting, Warsaw, Poland, September 18-21, 2023.

Two papers were published:

1. Mekhrdod S. Kurboniyon, Bibo Lou, Umar Zafari, Farhod Rahimi, Alok M. Srivastava, Tomoyuki Yamamoto, Mikhail G. Brik, Chong-Geng Ma, "*First-principles study of geometric and electronic structures, and optical transition energies of Mn^{4+} impurity ions: K_2SiF_6 as a prototype*", Journal of Luminescence 263 (2023) 120103.
2. Mekhrdod S. Kurboniyon, Umar Zafari, Chong-Geng Ma, Michal Piasecki, Mikhail G. Brik, and Tomoyuki Yamamoto, "*Geometrical and Electronic Structure Analysis of Mn-Doped $CaMO_3$(M=Ti, Zr, and Sn)*", Physica Status Solidi B 260 (2023) 2200575.