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Table of Content

Optical Materials, Volume 121, November 2021

Regular Articles

Spectroscopic studies of Cr3+ ions in natural single crystal of magnesium aluminate spinel MgAl2O4
N. Mironova-Ulmane, M.G. Brik, J. Grube, G. Krieke, ... A.I. Popov
Article 111496

An investigation of design principles toward near infrared organic upconversion devices
Wenli Lv, Juanjuan Zhou, Zhengkang Zhou, Xuan Li, ... Yingquan Peng
Article 111487

Enhanced visible and tunable infrared transmittance of W-doped VO2/SiO2/PVP composite films for smart windows
Jiran Liang, Shuangli Wang, Dangyuan Lei, Zhaoyang Wang, Xinzhe Li
Article 111485

Enhanced red emission in Li2Mg3TiO6: Mn4+ phosphor via Na+ and Ge4+ doping
Kai Ye, Zhiwen Yan, Xiaoliang Yang, Siguo Xiao
Article 111480

Investigation of dynamic optical study of Bi2Te3 topological insulators thin film based on MWCNT flexible paper using terahertz spectroscopy
Subhash Nimanpure, Animesh Pandey, Guruvandra Singh, Bhanu Pratap Singh, ... Mukesh Jewariya
Article 111490

The radioluminescence and photoluminescence behaviour of lithium alumino borate glasses doped with Tb2O3 and Gd2O3 for green luminescence applications
W. Rittisut, N. Wantana, Y. Ruangtaweep, P. Mool-am-kha, ... J. Kaewkhao
Article 111437

Specific complex-oxide crystals with strong nonlinear absorption and nonlinear refraction as promising optical materials
Dominique Guichaoua, Ihor Syvorotka, Ivan Solskii, Natalia Syvorotka, ... Bouchta Sahraoui
Article 111493

Theoretical analysis of effects of doping MAPbI3 into p-n homojunction on several types of perovskite solar cells
Quanmin He, Haiyan Gu, Dengqi Zhang, Guochuan Fang, Hanmin Tian
Article 111491

Influence of minority charge carrier lifetime and concentration on crystalline silicon solar cells based on double antireflection coating: A simulation study
Deb Kumar Shah, Devendra KC, Tae-Gwan Kim, M. Shaheer Akhtar, ... O-Bong Yang
Article 111500

Latest updates in growth and performance of Ce-doped Tl2LaCl5 and Tl2GdBr5 and Eu-doped TlCa2Br5 and TlSr2I5
R. Hawrami, E. Ariesanti, A. Burger, H. Parkhe
Article 111495

Influence of nanostructured SnS thin films for visible light photo detection
Devarajan Alagarasan, S. Varadharajaperumal, K. Deva Arun Kumar, R. Naik, ... R. Ganesan
Article 111489

Surface plasmon polaritons enhanced random lasing and weak localization of light in un- and ZnSe-coated Nd3+ doped (Pb,La)(Zr,Ti)O3 ceramics
Xinyan Ma, Zuoren Xiong, Yingbin Zhang, Hua Zhao
Article 111498

Comprehensive study of l-Alanine passivated colloidal gold nanoparticles and GNP-PVP thin films: Linear optical properties and very large nonlinear refractive index, absorption coefficient, third-order nonlinear susceptibility measurements and effect of passivation
A.L. Sunatkari, S.S. Talwatkar, Y.S. Tamgadge, G.G. Muley
Article 111458

Efficient surface enhanced Raman scattering substrates based on complex gold nanostructures formed by annealing sputtered gold thin films
Thi Huyen Trang Nguyen, Thi Mai Anh Nguyen, Cong Doanh Sai, Thi Hai Yen Le, ... Thi Ha Tran
Article 111488

Mushroom-structured silicon metasurface for broadband superabsorption from UV to NIR
Jinshuang Wu, Mingzhao Ouyang, Yu Zhao, Yeming Han, Yuegang Fu
Article 111504

Promoting photocatalytic performance of Bi2WO6 nanosheet incorporated with a 3D-Succulent plant-like SrMoO4 modified by Ag under simulated sunlight
Yufen Gu, Bobo Guo
Article 111473

AlN–Ce-doped yttrium aluminum garnet composite ceramic phosphor for high-power laser lighting
Kana Fujioka, Kenta Yagasaki, Takuya Sawada, Hisashi Minemoto, ... Kazuhisa Yamamoto
Article 111507

Densification, microstructure and optical properties of YAG transparent ceramics prepared by dry-pressing and gelcasting
Lan Chen, Yongzhi Luo, Yudong Xia, Bin Kang, Shengquan Yu
Article 111509

Nb–TiO2/P3HT hybrid solar cell: Oxide production and photovoltaic electrochemical characterization
Gideã Taques Tractz, Sandra Regina Masetto Antunes, Guilherme Arielo Rodrigues Maia, Henrique de Santana, ... Paulo Rogério Pinto Rodrigues
Article 111513

Low-order optical nonlinearities of PbS quantum dot liquids and films
R.A. Ganeev, I.A. Shuklov, A.I. Zvyagin, D.V. Dyomkin, ... V.F. Razumov
Article 111499

A new thermal degradation mechanism of red Sr2Si5N8:Eu phosphor: From the view of microstructural evolution
Xiong Yang, Xue-Jing Xing, Yi-Fan Liu, Chun-Hong Mu, ... Liang-Jun Yin
Article 111506

Stimulated overtone Raman scattering by polar modes in lithium tantalate
A. Yu. Pyatyshev
Article 111512

Effect of intrinsic point defects on the electronic and optical properties of Ho:BYF crystal
Lihong Han, Yuanyuan Zou, Jia Liu, Baonan Jia, ... Pengfei Lu
Article 111514

Enhanced thermal performance of photovoltaic panels based on glass surface texturization
Ángel Andueza, Cristina Pinto, David Navajas, Joaquín Sevilla
Article 111511

Preparation of fluorescent nitrogen-doped carbon dots for highly selective on-off detection of Fe3+ ions in real samples
Nazanin Hashemi, Mohammad H. Mousazadeh
Article 111515

Synthesis and modulation of multicolor fluorescent carbon dots from p-phenylenediamine and dansyl derivative for white light emitting diodes
L.B.O. Davi, D.J.P. Lima, C.D.A.E.S. Barbosa
Article 111502

Dependence of Judd-Ofelt parameters on overall changing factor of integrated absorption bands of Er3+

Mei-Hong Liu, Jia-Min Liu, Feng Chen, De-Long Zhang
Article 111477

Light scattering enhancement of ZnO nanorods via Mg–Al co-doping and their influence on polymeric photodetector
Tianfeng Weng, Miao Yan, Xuan Yu, Qian Qiao, ... Xiaoming Yu
Article 111516
Facile synthesis of visible-light-induced mesoporous Ag2O/Fe2(MoO4)3 photocatalysts for degradation of tetracycline
Adel A. Ismail, Soad Z. Alsheheri, Soha M. Albukhari, M.H.H. Mahmoud
Article 111505

Lattice induced transparency-like in symmetric metasurfaces tuned with incident angles in mid-infrared region
Yue Liang, Xiaofei Liu, Qi Han, Xueru Zhang, ... Yinglin Song
Article 111535

Design and analysis of a broadband metamaterial absorber applied to visible light band
Chenguang Zhang, Shijun Ji, Ji Zhao, Han Wu, Handa Dai
Article 111533

The nonlinear optical properties of nickel nano-films in the cw regime: Proposed model
Husam H. Abu-Safe, Razan Al-Esseili, Hussein Al-Taani, Husam El-Nasser, ... Morgan E. Ware
Article 111531

Optical, structural and electrical properties of sputtered ultrathin chromium films
Anna Sytchkova, Alexandr Belosludtsev, Lina Volosevičienė, Remigijus Juškėnas, Rimantas Simniškis
Article 111530

Polymer-nanoimprinting route for the construction of large-area Au@Ag plasmonic arrays using as highly-uniform SERS platforms
Wenkuan Che, Jing Wu, Mingfei Cheng, Lu Xu, Jinghuai Fang
Article 111532

Design and construction of diverse dual co-catalysts decorated Z-scheme g-C3N4/WO3(002) photocatalyst for converting nitrate and sulfite
Jianhe Tang, Yu Liu, Yitong Lin, Xueke Liu, ... Jun Wang
Article 111541

Acid@base co-sensitization strategy for highly efficient dye-sensitized solar cells
Yongliang Liu, Shengbo Zhu, Yilin Su, Ran Chen, ... Zhongwei An
Article 111528

Nitrogen, sulfur co-doped red carbon dots for sensitive and selective detection of Sn2+ ions
Peiyuan Zhu, Zhijun Zhu, Zhenhua Li, Yanan Xu, ... Jianguo Tang
Article 111543

Modulating visible-near-infrared reflectivity in ultrathin graphite by reversible Li-ion intercalation
Tao Liang, Gang Peng, Xiangzhe Zhang, Yuehua Wei, ... Xueao Zhang
Article 111517
Characterization broadband omnidirectional antireflection ITO nanorod films coating
T. Chaikeeree, N. Mungkung, N. Kasayapanand, T. Lertvanithphol, ... M. Horprathum
Article 111545

The effect of manganese (IV) oxide doping on the optical and elastic properties of calcium borate glass derived from waste chicken eggshell
A.S. Asyikin, A.A. Shamimi, S.N. Nazrin, M.K. Halimah, Imed Boukhris
Article 111540

Chromium nanostructures for enhancing light trapping in a thin-film solar cell
H. Rahimi, M.J. Karimi, S. Ghajarpour-Nobandegani
Article 111548

High performance nanohybrid CeO2@2D CdO plates with suppressed charge recombination: Insights of photoluminescence, visible-light photocatalysis, intrinsic mechanism and antibacterial activity
Asad Syed, Abdallah M. Elgorban, Abdulaziz A. Al Kheraif
Article 111510

Impact of pH on structural and sensing characteristics of cresol red encapsulated polyethylene glycol assisted silica nanomatrix: Sol-gel method
Shumaila Islam
Article 111546

Chromaticity coordinates of ruby based on first-principles calculation
Mega Novita, Irna Farikhah, Rizky Muliani Dwi Ujianti, Dian Marlina, ... Kazuyoshi Ogasawara
Article 111539

New strategy for improving the perovskite solar cells' open-circuit voltage: Cation substitution of hole transport layer
Xinshou Wang, Dongxing Kou, Canbin Ouyang, Jialei Liu
Article 111262

Improving the CRI of Al2O3-YAG:Ce eutectic for high-power white LEDs applications: Energy-transfer and co-luminescence
Hao Lu, Qingsong Song, Xiaodong Xu, Peng Liu, ... Yan Zhang
Article 111415

Synthesis and up-conversion luminescence properties of Ho3+-Yb3+ co-doped glass ceramics containing Sr3Gd(PO4)3
Tianli Zhao, Siying Wang, Xiangyu Zou, Hongbo Zhang, ... Chunhui Su
Article 111547

Structural, photoluminescence and Judd-Ofelt analysis of red-emitting Eu3+ doped strontium hexa-aluminate nanophosphors for lighting application
Priti Chaware, Amol Nande, S.J. Dhoble, K.G. Rewatkar
Article 111542

Perfect absorption in free-standing GaAs nanocylinder arrays by degenerate critical coupling
Wenya Chen, Xing Wang, Junyi Duan, Chaobiao Zhou, ... Shuyuan Xiao
Article 111558

Second harmonic generation in precisely diced KTiOAsO4 ridge waveguides
Genglin Li, Hui Xu, Yicun Yao, Yuechen Jia, Feng Chen
Article 111561

A comparative study of different rare-earth (Gd, Nd, and Sm) metals doped ZnO thin films and its room temperature ammonia gas sensor activity: Synthesis, characterization, and investigation on the impact of dopant
K. Kasirajan, L. Bruno Chandrasekar, S. Maheswari, M. Karunakaran, P. Shunmuga Sundaram
Article 111554

The effect of calcination temperature on the photophysical and mechanical properties of copper iodide (5 mol%)–doped hydroxyapatite
Sohrab Nasiri, Mozhgan Hosseinnezhad, Marzieh Rabiei, Arvydas Palevicius, Giedrius Janusas
Article 111559

Optically photoactive Cu–In–S@ZnS core-shell quantum dots/biopolymer sensitized TiO2 nanostructures for sunlight energy harvesting
Josué C. Amaral-Júnior, Alexandra A.P. Mansur, Isadora C. Carvalho, Herman S. Mansur
Article 111557

Wide-band EPR spectroscopy and relaxation study of Tm3+ ions in PbGa2S4 crystal
G.S. Shakurov, R.B. Zaripov, V.V. Badikov, D.V. Badikov
Article 111555

Influence of fluoroalkyl chains on structural, morphological, and optical properties of silica-based coatings on flexible substrate
Kamila Startek, Sebastian Arabasz, Alicja Bachmatiuk, Anna Lukowiak
Article 111524
Download PDF

Effect of aspect ratio of c-axis oriented ZnO nanorods on photoelectrochemical performance and photoconversion efficiency
Nikhil S K, Abinash Das, Mathan Kumar P, Muthuraaman Bhagavathiachari, Ranjith G. Nair
Article 111551

Towards high-efficiency planar heterojunction antimony sulfide solar cells
Hao Chen, Zhen-Qi Li, Bin Sun, Xiao-Dong Feng
Article 111556

All-dielectric water-based metamaterial absorber in terahertz domain
Feng Lan, Zi-Fan Meng, Jiu-Fu Ruan, Rui-Zhi Zou, Sheng-Wei Ji
Article 111572

Comparative study of quantum confinements effect present in Silicon Nanowires using absorption and Raman spectroscopy
Vikas Kashyap, Chandra Kumar, Neeru Chaudhary, Navdeep Goyal, Kapil Saxena
Article 111538

The influence of Ge substitution and H2S annealing on Cu2ZnSnS4 thin films
Canan Aytug Ava, Yusuf Selim Ocak, Sezai Asubay, Omer Celik
Article 111565

Structure and luminescent properties of Sm3+-doped metaphosphate glasses
Mohamed Atef Cherbib, Ismail Khattech, Habib Elhouichet
Article 111571

Effect of Tb3+ ion concentration on the up-conversion and down-conversion luminescence properties of the Yb3+/Ho3+/Tb3+ tri-doped SiO2–Al2O3–Y2O3–NaF–CaF2 glasses
Songxuan Liu, Zhiwei Luo, Ping Zhang, Weicheng Lei, ... Anxian Lu
Article 111567

Effect of solution pH on as-synthesized and calcined WO3 nanoparticles synthesized using sol-gel method
Mahboobeh Abbaspoor, Maryam Aliannezhadi, Fatemeh Shariatmadar Tehrani
Article 111552

Effects of particle size of raw materials on phase formation and optical properties of Ce3+-doped Y3Al5O12 phosphors
Shinnosuke Akiyama, Riho Moriyama, Junya Tanaka, Yasushi Sato, ... Hideki Kato
Article 111549

Suppressing the localized surface plasmon resonance of Ag nanoparticles to obtain ultra-high and ultra-uniform optical transmittance of dielectric-Ag-dielectric electrodes

Shuai Wang, Shiqi Zhao, Zhitao Cheng, Jie Wang, ... Yingcui Fang
Article 111569

Observation of negative photoconductivity at bandgap and super bandgap excitations in GaN nanorods
Shuchi Kaushik, Ashok Kumar Kapoor, Rohit Kumar Pant, Saluru Baba Krupanidhi, Rajendra Singh
Article 111553

Dy3+-doped lithium aluminoborate glass for luminescent light guides with high luminance
Michelle Grüne, Juliane Steinbrück, Stefan Schweizer
Article 111563
Download PDF

Improving backside (N-face) GaN substrate roughening by pre-annealing for GaN-on-GaN LED
Ezzah A. Alias, Norasmida Ibrahim, Steven P. DenBaars, Narong Chanlek, ... Norzaini Zainal
Article 111570

Temperature characteristics of Ge/ZnS one-dimension photonic crystal for infrared camouflage
Zichen Deng, Yarui Su, Wei Gong, Xian Wang, Rongzhou Gong
Article 111564

Broadband transparent terahertz vortex beam generator based on thermally tunable geometric metasurface
Qili Yang, Yan Wang, Lanju Liang, Maosheng Yang
Article 111574

1.53 μm luminescent properties of Er3+-doped fluoroaluminate glasses
V.A. Klinkov, E.A. Tsimerman, A.S. Rokhmin, V.D. Andreeva, ... A.N. Babkina
Article 111585

Investigation of defect, mechanical, thermal properties and refractive index on an Er:LuYSGG mixed laser crystal
Kunpeng Dong, Dunlu Sun, Huili Zhang, Jianqiao Luo, ... Shaotang Yin
Article 111568

A study of transmission on cylindrical photonic quasicrystals
J.A. Fernandes, D.H.A.L. Anselmo, M.S. Vasconcelos, V.D. Mello
Article 111566

Enhanced photodegradation of acid orange 61 by the novel hetero-junction CoFe2O4/AgCl
Billal Brahimi, Elhadj Mekatel, Mounir Mellal, Oussama Baaloudj, ... Mohamed Belmedani
Article 111576

Red, Green, Blue and IR emitting zirconium Titanate nano composite co-doped with Er3+/Tm3+/Yb3+ synthesized by combustion synthesis

A. Sangeetha, K.N. Sathish, B.M. Nagabhushana, Chikkahanumantharayappa, C.K. Jayasankar
Article 111534

Preparation of non-stoichiometric Gd2+xZr2O7+3x/2 transparent ceramics by vacuum sintering
Jianjun Zeng, Kuibao Zhang, Daimeng Chen, Ting Deng, ... Baozhu Luo
Article 111575

Graphene metasurface for broadband, wide-angle and polarization-insensitive carpet cloak
Pei Ding, Mingyu Li, Ximin Tian, Yan Li, ... Junqiao Wang
Article 111578

Synthesis of SERS imprinted membrane based on Ag/ESM with different morphologies for selective detection of antibiotics in aqueous sample
Guoqi Sui, Xiuyun Yang, Hongji Li, Yunhui Li, ... Shuo Dong
Article 111581

Influence of the size of Au nanoparticles on the photoinduced birefringence and diffraction efficiency of polarization holographic gratings in thin films of azopolymer nanocomposites
Nataliya Berberova-Buhova, Lian Nedelchev, Georgi Mateev, Elena Stoykova, ... Dimana Nazarova
Article 111560

Characterization of nanoparticulated WO3 electrochromic thin films prepared via precipitation reaction of peroxotungstic acid solution
Yoon-Tae Park, Ki-Tae Lee
Article 111577

Performance of sunlight responsive WO3/AgBr heterojunction photocatalyst toward degradation of Rhodamine B dye and ofloxacin antibiotic
Jirayus Piriyanon, Piyachat Takhai, Sireethorn Patta, Tammanoon Chankhanittha, ... Suwat Nanan
Article 111573

Performance analysis of carbon-based perovskite solar cells by graphene oxide as hole transport layer: Experimental and numerical simulation
Eri Widianto, Shobih, Erlyta Septa Rosa, Kuwat Triyana, ... Iman Santoso
Article 111584

Theoretical study by analytical equations of optical properties of the phosphors Zn2SnO4 codoped with Cr3+ and (Al3+ or Eu3+) via the crystal field control
Hajer Souissi, Olfa Taktak, Souha Kammoun
Article 111529

Emission-tunable Mn-doped ZnS/ZnO heterostructure nanobelts for UV-pump WLEDs
Do Quang Trung, Manh-Trung Tran, Nguyen Duy Hung, Quang Nguyen Van, ... Huy Pham Thanh

Article 111587

Influence of starting Y2O3 and Nd2O3 powders characteristics on optical properties of highly transparent Nd:Y2O3 ceramics
Hyeon-Myeong Oh, Ha-Neul Kim, Young-Jo Park, Jae-Woong Ko, Hyun-Kwuon Lee
Article 111562

Strong optical non-reciprocity in one-dimensional photonic crystal containing a Weyl semimetal-based defect
Tianming Li, Chengping Yin, Feng Wu
Article 111583

Forming laterally structured heterojunction with FAPbI3 film for improving performance of MAPbBr3 photodetectors
Minmin Zhang, Wu Lifang, Shunfa Gong, Qiuju Han, Wenzhi Wu
Article 111586

Impact of fluorination on photovoltaic performance in high thermo- and photo-stability perylene diimide-based nonfullerene small molecular acceptors
Junfeng Tong, Xuefeng Jiang, Honglin Li, Lili An, ... Yangjun Xia
Article 111593

MgFe2O4 decoration of g-C3N4 nanosheets to enhance CIP oxidation in visible-light photocatalysis
Mohammad W. Kadi, Reda M. Mohamed, Detlef W. Bahnemann
Article 111598

Scintillation characteristics and temperature quenching of radio- and photoluminescence of Mg2+-codoped (Lu,Gd)3Al2.4Ga2.6O12:Ce garnet crystals
Warut Chewpraditkul, Nakarin Pattanaboonmee, Ongsa Sakthong, Weerapong Chewpraditkul, ... Martin Nikl
Article 111595

Experimental and theoretical analysis of radiation shielding properties of strontium-borate-tellurite glasses
Dalal Abdullah Aloraini, Aljawhara H. Almuqrin, M.I. Sayyed, Ashok Kumar, ... A.V. Trukhanov
Article 111589

Impacts of both temperature and condensation on the band gap of photonic crystals around the freezing point
Yen-Hsiang Chen, Yu-Jung Lu, Jui-Yung Chang, Yu-Bin Chen
Article 111596

Solvothermal synthesis and upconversion properties in Yb3+/Ln3+ (Ln3+=Er3+/ Ho3+/ Tm3+) codoped In2O3 nanoparticles with fine stability

Yuchao Shi, Jing Li, Wenhao Cui, Yaru Peng, ... Li Chen
Article 111601

Promoting effect of cellulose-based carbon dots at different concentrations on multifunctional photocatalytic degradation of dyes by ZnO
Shaopeng Li, Xueqi Chen, Zhuoying Cheng, Suyue Luo, ... Xing Gao
Article 111591

Active control of plasmon-induced transparency based on a GaAs/Si heterojunction in the terahertz range
Dan Li, Chunya Luo, Huaixing Wang, Furi Ling, Jianquan Yao
Article 111609

Preparation of chiral polymer/cholesteric liquid crystals composite films with broadband reflective capability for smart windows and thermal management of buildings
Huimin Zhang, Ping Yu, Tingjun Zhong, Yuzhen Zhao, ... Wenbo Shen
Article 111611

Citric acid modulated preparation of CdS photocatalyst for efficient removal of Cr(VI) and methyl orange
Jian Guan, Zeqing Long, Qiangang Li, Jinchi Han, ... Guangming Zhang
Article 111604

Structural and Optical Properties of Ultra-thin g-C3N4 nanotubes based g-C3N4/Ag/Ag2CrO4 ternary composite photocatalyst with Z-scheme carrier transfer mechanism
Fucheng Yu, Junpeng Cui, Yadong Zhou, Yuanmeng Li, ... Yangshuo Liu
Article 111608

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Research Article

Chromaticity coordinates of ruby based on first-principles calculation

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ABSTRACT

Understanding the local atomic configuration is crucial for studying phosphor materials. Their performance in many applications is strongly dependent upon their optical properties. Much experimental and theoretical effort has been made to meet the requirements. Specifically, *ab-initio* studies have extensively reported the absorption spectra and the multiplet energies of phosphors. However, the qualitative analysis on the emitted light has not yet been reported. In this work, we characterized the emitted light of ruby, which is a widely studied phosphor material. The absorption spectra of ruby were calculated utilizing the non-empirical discrete variational Xα (DV-Xα) and discrete variational multi-electron (DVME) software. Then, the investigation on the (*x*,*y*) chromaticity coordinates of was performed under the standard illuminant D65 utilizing ColorAC software, a chromaticity diagram maker. In this work, we used a ruby model cluster generated from an α-Al_2O_3 crystal. The model consists of seven atoms, where one chromium atom surrounded by six oxygen atoms. We compared the absorption spectra obtained via simple configuration interaction (CI) and those obtained which include energy corrections called configuration dependent correction (CDC) and correlation correction (CC). We successfully reproduced the color that is observed in experiment. The chromaticity coordinates approach red region for higher concentration. The results show that the calculation with CDC-CC shows better agreement with experiment. This research confirms the non-empirical calculations based on the DV-Xα and DVME methods, in the terms of emitted light.

1. Introduction

In the study of phosphor materials, it is very important to understand the local atomic arrangement. The quantum mechanical calculations, also known as first-principles calculations, have therefore gained increased importance not only for deep understanding of various basic properties of materials, but also for design and development of many kinds of new phosphor materials. For several decades, the density functional theory (DFT) calculation method has been employed to solve various problems in material science [1,2]. Various DFT methods have been shown to be very useful for the calculation of molecular orbital and band structure calculations including discrete variational Xα (DV-Xα) method [3–5], plane wave basis pseudopotential (PWPP) [6,7], full potential linearized augmented plane wave (FLAPW) method [8], and Orthogonalized Linear Combination of Atomic Orbitals (OLCAO) method [9–11].

The transitions between multiplets of the impurity states of phosphor materials play an important role in the luminescent process. Basically, these multiplets are determined by the local structure of the material. In order to correctly assign the multiplets from the experiment, accurate information on electronic state and chemical bonding is needed. Unfortunately, there are some difficulties which cannot be solved by the above theoretical approaches. Ordinary DFT calculations based on one-electron methods could not directly calculate the multiplets; therefore, first-principles many-electron calculations i.e. configuration interaction (CI) method should be employed to solve this type of problem. To calculate multiplet states of transition-metal ions in crystals, Ogasawara et al. [12–16] created discrete variational multi-electron (DVME) software, which is based on DV-Xα molecular orbital (MO) method. This method has been used effectively on a series of crystals doped with either rare earth or transition metal ions [17–27]. Although multiplets can be directly calculated in simple CI calculations, those energies are

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generally overestimated. On the other hand, although the average energy of multiplets can be well reproduced in a DFT calculation, the multiplets cannot be directly calculated. To decrease the overestimation, CI calculations with corrections based on one-electron DFT calculations were introduced. Even if the theoretical and the observed spectra are more closely aligned when CI is coupled with corrections, the qualitative color reproduced by the theoretical phosphor material is not clear.

In the eye, there are three different types of cones: S, M, and L. The S-cones are responsible for short-wavelength sensitivity, the M-cones for middle-wavelength sensitivity, and the L-cones for long-wavelength sensitivity. This means that the human eye is only capable of detecting red, green, and blue and the brain then extrapolates all other colors based on the intensities of the original three colors. In the 1920s, William David Wright and the International Commission on Illumination (CIE) set out to measure the wavelength sensitivity of each of these cones developing the CIE standard observer color matching functions and the color space chromaticity diagram [28,29]. With this information, it became possible to qualitatively measure the color of an object as perceived by a standard observer for the first time. This event is regarded as the beginning of colorimetry.

According to the science of colors, chromaticity is one of the common color parameters used for characterization the emitted light. It can be calculated from the absorption spectrum. The most widely-used model comes from the Commission Internationale d'Eclairage (CIE 1931) [30–32]. As the name implies, the chromaticity diagram is an array of potential colors. Each color is specified by a pair of a numerical coordinates, called the chromaticity coordinate. We may use the chromaticity diagram to show how different hues of light mix together. The pure spectral hues of the rainbow are represented by the points on the curved border. Note that any color inside the diagram can be made in different ways, and only colors around the edge of the diagram are unique colors.

For about a decade, we have been studied the optical properties of ruby, such as lattice relaxation effect, molecular orbitals, multiplet energies, absorption spectra, and pressure dependence, [19–21]. Although non-empirical studies have been conducted, qualitative analysis of the emitted light has not been reported. Therefore, in this work, we characterized the emitted light of ruby. The absorption spectra of ruby were calculated with the non-empirical DV-Xα and DVME software. Then, the (x, y) chromaticity coordinates were investigated using ColorAC software. This research is important in confirming the non-empirical characterization of emitted light based on the DV-Xα and DVME methods.

2. Computational procedure

As illustrated in Fig. 1, seven-atom model clusters were built on a host α-Al_2O_3 crystal with Rh_2O_3 structure [33]. To generate the effective Madelung potential, a Cr^{3+} ion was placed in the cluster's core and approximately 13,600-point charges were placed at the outer atomic sites of the cluster. The local structure of the cluster (C_3 symmetry) was preserved during the calculation; 20,000 sample points were used.

Because the DVME technique is discussed in its entirety in Ref. [14], only the mathematical formulation required to understand the results in this study is explained. We first calculated the molecular orbital using the one-electron DV-Xα method, followed by the optical spectra calculations using the many-electron CI calculations as the main core of the DVME method.

In the one-electron calculations, only one electron is considered. The interaction with the other electrons are averaged and treated just as a potential. The Schrödinger equation for the one-electron calculation is expressed as

$$h\psi(\boldsymbol{r}) = \varepsilon\psi(\boldsymbol{r}) \tag{1}$$

The one-electron Hamiltonian is expressed as

$$h(\boldsymbol{r}) = -\frac{1}{2}\nabla^2 + V(\boldsymbol{r}) \tag{2}$$

The effective molecular potential $V(\boldsymbol{r})$ is expressed as

$$V(\boldsymbol{r}) = -\sum_v \frac{Z_v}{|\boldsymbol{r}-\boldsymbol{R}_v|} + \int \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}'-\boldsymbol{r}|}d\boldsymbol{r}' + V_{xc}\{\rho(\boldsymbol{r})\} - 3\alpha\left\{\frac{3}{8\pi}\rho(\boldsymbol{r})\right\}^{1/3} \tag{3}$$

where α is 0.7 and the electron density $\rho(\boldsymbol{r})$ is given by

$$\rho(\boldsymbol{r}) = \sum_l \rho_l(\boldsymbol{r}) = \sum_l f_l|\varphi_l(\boldsymbol{r})|^2 \tag{4}$$

where f_l is the occupancy.

The Schrödinger equation for many-electron calculation is expressed

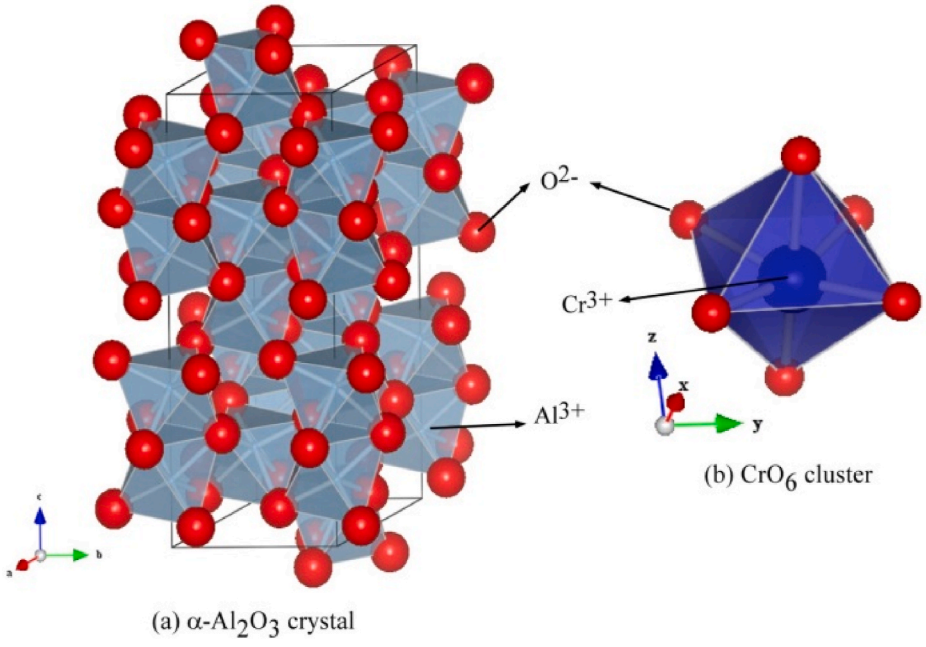

Fig. 1. (a) α-Al_2O_3 crystal structure obtained from Sawada et al. [33] and (b) CrO_6 model cluster used in the calculations.

as

$$H\Psi_l = E\Psi_l \tag{5}$$

Here, electron-electron interactions are directly calculated. The many-electron wave function is expressed as

$$\Psi_l = \sum_{j=1}^{N} W_{jl}\Phi_j \tag{6}$$

W_{jl} is the coefficient of the Slater determinants (Φ_j) used in this calculation, which is expressed as

$$\Phi_j(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \varphi_{j1}(\boldsymbol{r}_1) & \varphi_{j1}(\boldsymbol{r}_2) & \cdots & \varphi_{j1}(\boldsymbol{r}_n) \\ \varphi_{j2}(\boldsymbol{r}_1) & \varphi_{j2}(\boldsymbol{r}_2) & \cdots & \varphi_{j2}(\boldsymbol{r}_n) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{jn}(\boldsymbol{r}_1) & \varphi_{jn}(\boldsymbol{r}_2) & \cdots & \varphi_{jn}(\boldsymbol{r}_n) \end{vmatrix} \tag{7}$$

Here, r denotes the electron's location. φ_j's are the molecular orbitals that mostly consist of TM 3d orbitals generated from DV-Xα MO calculations. The effective many-electron Hamiltonian for explicitly treated N electrons is written as

$$H = \sum_{i=1}^{N} h(\mathbf{r}_i) + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}}, \tag{8}$$

where r_{ij} denotes the distance between the ith electron and the jth electron, and h denotes the one-electron operators, which may be written as

$$h(\mathbf{r}_i) = -\frac{1}{2}\nabla_i{}^2 + V_{nuc}(\mathrm{r}_i) + V_0(\mathrm{r}_i). \tag{9}$$

V_{nuc} denotes the potential owing to the nuclei, whereas V_0 denotes the potential due to the other electrons. As a results, only electrons occupying impurity levels are specifically handled in this calculation. The effective many-electron Hamiltonian can be expanded as follows:

$$\Phi_p|H|\Phi_q = \sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}^{pq} i|h|j + \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} B_{ijkl}^{pq} ij|g|kl, \tag{10}$$

H is then diagonalized inside the subspace spanned by the Slater determinants Φ_i derived from the impurity-state orbitals obtained from the one-electron MO calculations. This step was performed to get the many-electron wave functions and multiplet energies. The many-electron wave functions for each multiplet state may be explicitly calculated as a linear combination of the Slater determinants using the eigenvector obtained by the diagonalized many-electron Hamiltonian. As a result, we can simply calculate the oscillator strength for the electric-dipole transition (transition probability) between multiplets by

$$I_{if} = 2\left(E_f - E_i\right)\left|\Psi_i\left|\sum_{k=1}^{N} \mathrm{r}_k.\mathrm{e}\right|\Psi_f\right|^2 \tag{11}$$

Here, the initial and final states of the many-electron wave functions are denoted by Ψ_i and Ψ_f. Whereas the energy eigenvalues of these states are denoted by E_i and E_f. The unit vector parallel to the direction of the incoming light's electric field is represented by e.

Multiplet energies obtained from many-electron CI calculations are usually underestimated because of the 10–50% overestimation of crystal field splitting [34]. In order to enhance the accuracy of theoretical multiplet energies, numerous adjustments such as configuration dependency correction (CDC) and correlation correction (CC) are considered. In the CDC approach, the barycenters of $(t_{2g})^3$, $(t_{2g})^2(e_g)^1$, $(t_{2g})^1(e_g)^2$, and $(e_g)^3$ configurations were adjusted to be 0, $10Dq$, $20Dq$, and $30Dq$, respectively. Here, the crystal field splitting $10Dq$ was determined using the spin-restricted one-electron MO calculation. On the other hand, in the CC approach, the factor c was calculated from first-principle calculations based on the consistency of the transition energy of the spin-flip transition from $(t_{2g}\uparrow)^3$ to $(t_{2g}\uparrow)^2(t_{2g}\downarrow)^1$ between the many electron CI calculations and the spin-unrestricted one-electron MO calculations. The Hamiltonian with CDC correction is written as

$$\Phi_p\left|H^{CDC}\right|\Phi_q = \sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}^{pq} i|h|j + \sum_{i=1}^{L}\sum_{j=1}^{L}\sum_{k=1}^{L}\sum_{l=1}^{L} B_{ijkl}^{pq} ij|g|kl + D_{CDC}(m,n)\delta_{pq} \tag{12}$$

where (m,n) denotes the value for $(t_{2g})^m(e_g)^n$ configuration. On the other hand, the Hamiltonian with CC correction is written as

$$\Phi_p\left|H^{CC}\right|\Phi_q = \sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}^{pq} i|h|j + \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} c \times B_{ijkl}^{pq} ij|g|kl \tag{13}$$

In this case, the effective Hamiltonian including the CDC and CC effects, is written as

$$\Phi_p\left|H^{CDC-CC}\right|\Phi_q = \sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}^{pq} i|h|j + \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} c \times B_{ijkl}^{pq} ij|g|kl + D_{CDC}(m,n)\delta_{pq} \tag{14}$$

In order to analyze the color parameters, the CIE 1931 chromaticity diagram in the ColorAC software is used. The emitted light's color is represented by x and y graph coordinates. This graph is expressed as a red, green, and blue color ratio. These three colors are the X, Y, Z tristimulus values; they correspond to the band-pass filtered chromaticity response of cones in the human retina. The chromaticity coordinates were calculated based on the transmittance which is obtained from absorbance. Transmittance can be defined by

$$T(\lambda) = \frac{I(\lambda)}{I_0(\lambda)} \tag{15}$$

where I_0 is the intensity of incident light while I is that of transmitted light. On the other hand, absorbance can be defined by

$$A(\lambda) = -\log\left(\frac{I(\lambda)}{I_0(\lambda)}\right) \tag{16}$$

Therefore, the transmittance can be calculated by

$$T(\lambda) = e^{-A(\lambda)} \tag{17}$$

Then X, Y, Z can be expressed as

$$\begin{aligned} X &= \int_{380}^{780} T(\lambda)P(\lambda)\overline{x}(\lambda)d\lambda = \int_{380}^{780} e^{-A(\lambda)}P(\lambda)\overline{x}(\lambda)d\lambda \\ Y &= \int_{380}^{780} T(\lambda)P(\lambda)\overline{y}(\lambda)d\lambda = \int_{380}^{780} e^{-A(\lambda)}P(\lambda)\overline{y}(\lambda)d\lambda \\ Z &= \int_{380}^{780} T(\lambda)P(\lambda)\overline{z}(\lambda)d\lambda = \int_{380}^{780} e^{-A(\lambda)}P(\lambda)\overline{z}(\lambda)d\lambda \end{aligned} \tag{18}$$

Here $P(\lambda)$ denotes the standard illuminant D65, which represents natural daylight. Generally, the absorbance is proportional to the molar absorption coefficient ε, the molar concentration of the particles (in this case, chromium ions) c, and the sample thickness l.

$$A(\lambda) = \varepsilon(\lambda)cl \tag{19}$$

Therefore a multiplication of the absorbance by a scalar such as $A_2 = aA_1(\lambda)$ means that the concentration and/or the sample thickness are changed so that $c_2l_2 = ac_1l_1$ is satisfied. Finally, the (x, y) chromaticity coordinates may be derived by

$$x = \frac{X}{X+Y+Z}$$
$$y = \frac{Y}{X+Y+Z} \quad (20)$$

3. Results and discussion

The experimental d-d absorption spectra of ruby published by Fairbank et al. [35] are shown in Fig. 2 together with two theoretical spectra derived from CI calculations without and with CDC-CC correction. The π spectra are represented by solid lines, whereas the σ spectra are represented by dashed lines. The three broad peaks in the measured spectra are assigned as the transition energies from the $^4A_2$ ground state to $^4T_2$, $^4T_{1a}$, and $^4T_{1b}$ states, respectively. It is well-known that these transition energies are generally noted as U-, Y- and Y′- bands, respectively. If we compare the spectra of U-band energy, the σ spectrum is higher than the π spectrum. The situation is opposite for Y- and Y′-band energies. The peak positions of U-, Y-, and Y′-bands are at ~2.2, ~3.0, and ~4.8 eV, respectively. Nevertheless, the peak position in each peak differs slightly between the σ spectrum and the π spectrum.

The three broad peaks and absolute intensities were successfully reproduced in the theoretical spectra. The U-, Y-, and Y′-bands of uncorrected calculations were found at ~2.5, ~3.7 and ~5.7 eV. When the CDC-CC correction was applied, those peaks moved to lower energies at ~2.3, ~3.3 and ~5.0 eV, respectively. The estimated peak positions were enhanced using CDC-CC correction.

Previously, several calculations on ruby have been performed. In 2000, Prof. Ogasawara's group [14] calculated ruby model clusters consisting of 41, 63 and 111 atoms. The TM ion was positioned in the middle of each cluster. In those clusters, 7, 14, and 26 Al ions were included. The effect of structural relaxation was considered by adopting the results of Kizler's extended X-ray absorption fine structure (EXAFS) [36]. They also considered the CDC-CC correction to improve the accuracy. We have also performed calculations with a ruby model cluster consisting of 63 atoms [19]. Although we treated the cluster similar to Ref. 9, several computation conditions such as the external atomic sites used to produce Madelung potentials and the sample points were different.

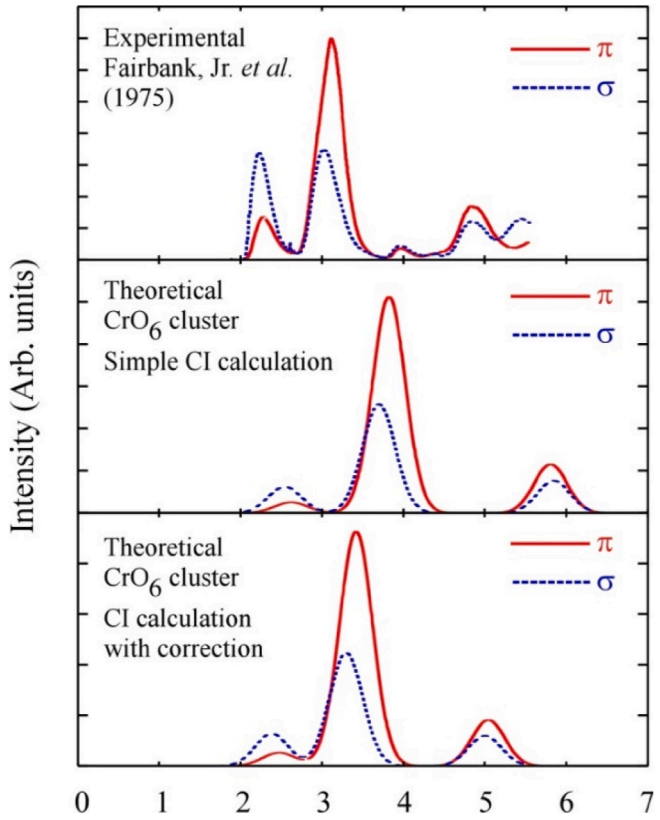

Fig. 2. Experimental and theoretical spectra of ruby (α-Al_2O_3: Cr^{3+}). The experimental spectra were obtained from Fairbank et al. [35] whereas the theoretical spectra were obtained from CI calculations without and with CDC-CC correction using CrO_6 cluster.

Table 1 shows the comparison of U-, Y- and Y′- bands peak position. As we can see, all of the computational results (except for the results from the simple CI calculation) show good agreement with the experimental data provided by Fairbank et al. [35]. The variation between the current and previous results is very small. However, simple CI calculations overestimated the U-, Y-, and Y′-bands' peak position. These findings imply that simple CI calculations with CDC-CC correction is a good method for accurately predicting the absorption spectra of ruby.

Therefore, based on the absorption spectra obtained in Fig. 2, we then evaluate the (*x*,*y*) chromaticity coordinates. It was performed under the standard illuminant D65 obtained from the experimental spectra and the theoretical spectra of CrO_6 cluster that are shown in Fig. 3. The chromaticity coordinates obtained from the experimental spectra are shown by a circle (●); the chromaticity coordinates obtained from theoretical spectra are shown by a triangle (▼); and a square (■) is used to denote CI calculations without and with considering CDC-CC correction. Since the color depends on conditions such as Cr^{3+} concentration and sample thickness and/or density, several points corresponding to different conditions were calculated and plotted. The "experimental color" approaches red for higher concentration. In our calculations, the "theoretical color" obtained without and with considering CDC-CC correction reproduced the same tendency. However, in the case of the CI calculation with CDC-CC corrections, the agreement between the theoretical color and the experimental color is quite good. It indicates that a CI calculation with CDC-CC correction effectively reproduces the absorption spectra of transition metal ions in crystals.

4. Conclusion

The theoretical absorption spectra of ruby were used to compute its chromaticity coordinates under the standard illumination D65. We began by calculating theoretical absorbance spectra with the first-principles DVME technique. The detailed comparison indicates that when CDC-CC correction is considered, the accuracy of the theoretical spectra are considerably enhanced. The numbers of peak, relative intensity between π and σ spectra, as well as the peak positions were well-reproduced in our calculation. These were then displayed on the CIE 1931 color space to get chromaticity coordinates. Next, the result was compared to the experimental data. The higher the concentration, the closer the chromaticity coordinates are to red. The estimated chromaticity coordinates for the spectra obtained by the CI calculation with CDC-CC corrections correspond well with the observed values. Therefore, on the basis of chromaticity coordinates, the agreement between the theoretical spectrum and the experimental spectrum has been quantitatively assessed.

Table 1
The peak position of U-, Y- and Y′- bands of observed spectra and the theoretical spectra.

	U-band (eV)		Y-band (eV)		Y′-band (eV)	
	π	σ	π	σ	π	σ
Expt [35]	2.24	2.27	3.03	3.11	4.85	4.82
Ogasawara [14]	2.31	2.46	3.24	3.40	4.95	4.94
Novita [19]	2.20	2.12	3.17	3.00	4.61	4.60
Simple CI	2.56	2.52	3.80	3.65	5.73	5.81
CI with correction	2.39	2.34	3.42	3.29	5.02	5.05

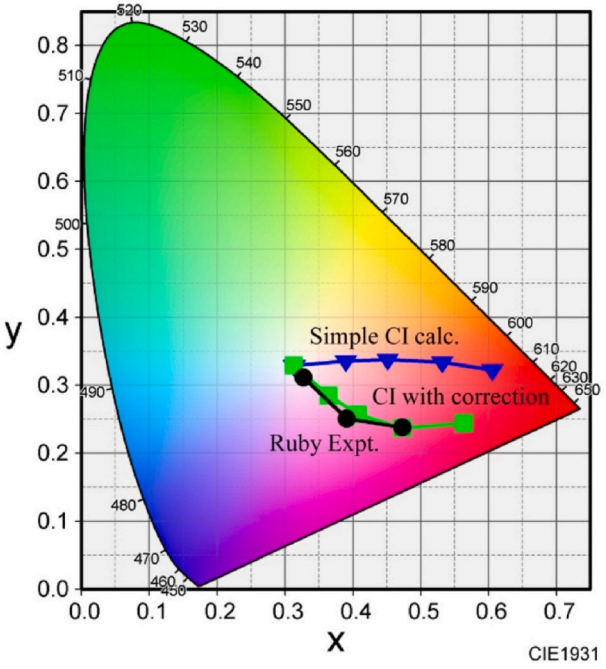

Fig. 3. Chromaticity diagram of experimental and theoretical color coordinates of ruby (α-Al_2O_3: Cr^{3+}). Ruby's experimental data derived from Fairbank's spectra (●) [35]; theoretical absorption spectra obtained from CI calculations without (▾) and with (■) CDC-CC correction using CrO_6 cluster are compared. Various concentrations of Cr^{3+} are represented by points placed along the lines.

Credit authorship contribution statement

Mega Novita: Conceptualization, Methodology, Writing – original draft, Writing – review & editing, Draft. **Irna Farikha:** Investigation, Resources. **Rizky Muliani Dwi Ujianti:** Project administration. **Dian Marlina:** Writing – original draft, Visualization. **Benjamin Walker:** Writing – review & editing, Draft, Proofread. **Hironori Kiyooka:** Visualization. **Shota Takemura:** Data curation, Proofread. **Kazuyoshi Ogasawara:** Supervision, Software, Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Mega Novita <novita@upgris.ac.id>

Your Submission OM-D-21-01962R1

1 pesan

Alok M Srivastava <em@editorialmanager.com> 30 Agustus 2021 13.59
Balas Ke: Alok M Srivastava <srivastaam@outlook.com>
Kepada: Mega Novita <novita@upgris.ac.id>

Ms. Ref. No.: OM-D-21-01962R1
Title: Chromaticity Coordinates of Ruby based on First-Principles Calculation
Optical Materials

Dear Dr. Mega Novita,

I am pleased to inform you that I have sent your paper to production.

Elsevier will contact you shortly with publication details.

Thank you for submitting your work to Optical Materials.

Yours sincerely,

Aravind Somasundaram
Data Administrator [25-May-2015]
Optical Materials

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Mega Novita <novita@upgris.ac.id>

Your Submission

1 pesan

Alok M Srivastava <em@editorialmanager.com> 18 Agustus 2021 18.40
Balas Ke: Alok M Srivastava <srivastaam@outlook.com>
Kepada: Mega Novita <novita@upgris.ac.id>

Ms. Ref. No.: OM-D-21-01962
Title: Chromaticity Coordinates of Ruby based on First-Principles Calculation
Optical Materials

Dear Dr. Mega Novita,

The reviewers have commented on your above paper. They indicated that it is not acceptable for publication in its present form.

However, if you feel that you can suitably address the reviewers' comments (included below), I invite you to revise and resubmit your manuscript within 20 days of this letter.

If we will have to extend this deadline, please let us know in time, as your article will be removed from the system when the dealine is reached.
After this you will have to submit your article again as a new one.

Please carefully address the issues raised in the comments.

If you are submitting a revised manuscript, please also:

a) outline each change made (point by point) as raised in the reviewer comments

AND/OR

b) provide a suitable rebuttal to each reviewer comment not addressed

Please be aware that the revised manuscript can be shown to the same or other referees.

To submit your revision, please do the following:

1. Go to: https://www.editorialmanager.com/om/

2. Enter your login details

3. Click [Author Login]
This takes you to the Author Main Menu.

4. Click [Submissions Needing Revision]

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I look forward to receiving your revised manuscript.

Yours sincerely,

Alok M Srivastava
Editor
Optical Materials

Reviewers' comments:

COMMENTS FROM EDITOR (Dr. Alok M Srivastava , Editor) AND REVIEWERS

Reviewer #1: A very interesting paper, which addresses theoretical calculations of the chromaticity coordinates. I would recommend the manuscript to be revised before it can be published.
1. English must be revised thoroughly. Even in the highlights there are grammar mistakes (plural and singular forms, verbs, ...). There are also many similar mistakes in the text, e.g. "is strongly depends" ("is" to be removed here) " Many
experimental and theoretical effort" ("many efforts" or "much effort"), "C3 symmetry, was preserve " ("was preserved"), etc - please, do check the whole manuscript!
2. In Eq. (15) the T(lambda) function is written to be transmittance. The authors calculated absorption spectra; please, explain in more details what in fact was used for the chromaticity coordinates calculations.

*****

Data in Brief (optional):

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Mega Novita <novita@upgris.ac.id>

Your Submission

1 pesan

Optical Materials <em@editorialmanager.com> 30 Agustus 2021 02.12
Balas Ke: Optical Materials <support@elsevier.com>
Kepada: Mega Novita <novita@upgris.ac.id>

Ms. Ref. No.: OM-D-21-01962R1
Title: Chromaticity Coordinates of Ruby based on First-Principles Calculation
Optical Materials

Dear Dr. Novita,

I am pleased to inform you that your paper "Chromaticity Coordinates of Ruby based on First-Principles Calculation" has been accepted for publication in Optical Materials. Depending on the journal that you have chosen during the submission process, we will ensure that we process your paper in the correct journal.

Below are comments from the editor and reviewers.

Thank you for submitting your work to Optical Materials.

With kind regards,

Alok M Srivastava
Editor
Optical Materials

Comments from the editors and reviewers:

Reviewer #1: The authors took into account my recommendations, the manuscript has been improved and can be accepted in its revised form.

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Submission Confirmation for OM-D-21-01962R1

1 pesan

Alok M Srivastava <em@editorialmanager.com> 26 Agustus 2021 21.46
Balas Ke: Alok M Srivastava <srivastaam@outlook.com>
Kepada: Mega Novita <novita@upgris.ac.id>

Ms. Ref. No.: OM-D-21-01962R1
Title: Chromaticity Coordinates of Ruby based on First-Principles Calculation
Original research article
Optical Materials

Dear Dr. Mega Novita,

This message is to acknowledge that we have received your revised manuscript for reconsideration for publication in Optical Materials.

You may check the status of your manuscript by logging into the Editorial Manager as an author at https://www.editorialmanager.com/om/.

Thank you for submitting your work to Optical Materials.

Kind regards,

Editorial Manager
Optical Materials

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Mega Novita <novita@upgris.ac.id>

Editor handles your revised submission OM-D-21-01962R1

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Optical Materials <em@editorialmanager.com> 27 Agustus 2021 14.26
Balas Ke: Optical Materials <support@elsevier.com>
Kepada: Mega Novita <novita@upgris.ac.id>

Ref.: Revision of OM-D-21-01962R1
Title: Chromaticity Coordinates of Ruby based on First-Principles Calculation

Dear Dr. Novita,

Your revised submission "Chromaticity Coordinates of Ruby based on First-Principles Calculation" will be handled by Editor Alok M Srivastava.

You may check the progress of your revision by logging into the Editorial Manager as an author at https://www.editorialmanager.com/om/.

Thank you for submitting your revision to this journal.

Kind regards,

Editorial Manager
Optical Materials

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Share your article [OPTMAT_111539] published in Optical Materials

1 pesan

Elsevier - Article Status <Article_Status@elsevier.com> 30 September 2021 16.17
Kepada: novita@upgris.ac.id

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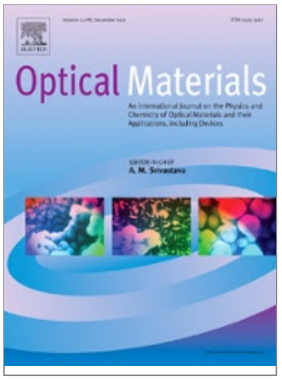
Share your article!

Dear Dr. Novita,

We are pleased to let you know that the final version of your article *Chromaticity Coordinates of Ruby based on First-Principles Calculation* is now available online, containing full bibliographic details.



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Order offprints of your article [OPTMAT_111539]

1 pesan

Elsevier - Offprints <Article_Status@elsevier.com> 11 November 2021 04.31
Kepada: novita@upgris.ac.id

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Dear Dr. Novita,

We would like to remind you of the option to order offprints of your article Chromaticity Coordinates of Ruby based on First-Principles Calculation.

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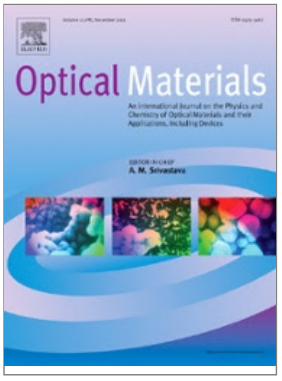
Kind regards,
Elsevier Author Support



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Article tracking [OPTMAT_111539] - Printed journal dispatched to subscribers

1 pesan

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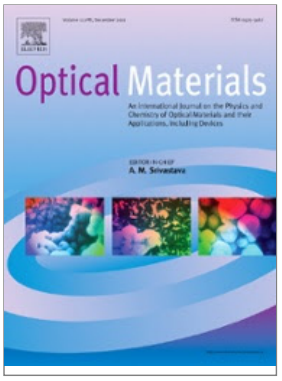
Journals dispatch

Dear Dr. Novita,

The printed journal issue which includes your article titled *Chromaticity Coordinates of Ruby based on First-Principles Calculation* in the journal *Optical Materials*, will be dispatched to subscribers on 22-NOVEMBER-2021



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