



## 山本 知之 Tomoyuki YAMAMOTO

TEL : 03-5286-3317 FAX : 03-5286-3317

e-mail : tymmt@waseda.jp

URL : <http://www.cms.sci.waseda.ac.jp>

1993年早稲田大学理工学部材料工学科卒業、1997年－1999年同各務記念材料技術研究所助手、1998年同理工学研究科材料工学専攻博士後期課程修了（博士（工学））、1999年－2002年理化学研究所研究員、2002年－2005年京都大学大学院工学研究科研究員、2005年－2010年早稲田大学理工学部助教授（2007年より准教授）、2010年－同教授、2018年同材料技術研究所兼任研究員、2019年－同拠点研究員

B.E. (1998, Waseda Univ.), Research Associate at Waseda Univ. (1997-1999), Ph.D. (1998, Waseda Univ.), Researcher at RIKEN (1999-2002), Researcher at Kyoto Univ. (2002-2005), Associate Prof. at Waseda Univ. (2005-2010), Prof. at Waseda Univ. (2010-)

材料の電気的、磁氣的、光学的などの物性に関して、量子力学を用いて原子レベルのミクロな視点に立ち、特に、極微量な添加元素や欠陥導入による機能発現機構の解明と、それらの知見に基づく新規機能性材料創製を目指した基礎研究を進めています。その中でも近年特に、“光と物質の相互作用”に焦点を絞り、希土類フリー蛍光体、アップコンバージョン蛍光体、有機無機ハイブリッドペロブスカイトを用いた次世代太陽電池などを対象として、シンクロトロン放射光を用いたX線分光や電子分光などの先端分析や、第一原理計算を用いた電子状態解析を進めています。

Basic researches on the materials properties, such as electronic, magnetic and optical properties, have been carried out at an atomic level in microscopic view point by using the quantum mechanics. Especially mechanism of newly appeared functions by dilute doping is studied, on whose knowledge new functional materials have been developed. Focusing upon the “interaction between light and matter” in these years, cutting-edge X-ray and electron spectroscopies using synchrotron radiations and first-principles electronic structure calculations have been conducted for various kinds of functional materials, e.g., rare-earth free red-emitting phosphors, up-conversion type phosphors, and next generation solar cells with organic-inorganic hybrid perovskite.

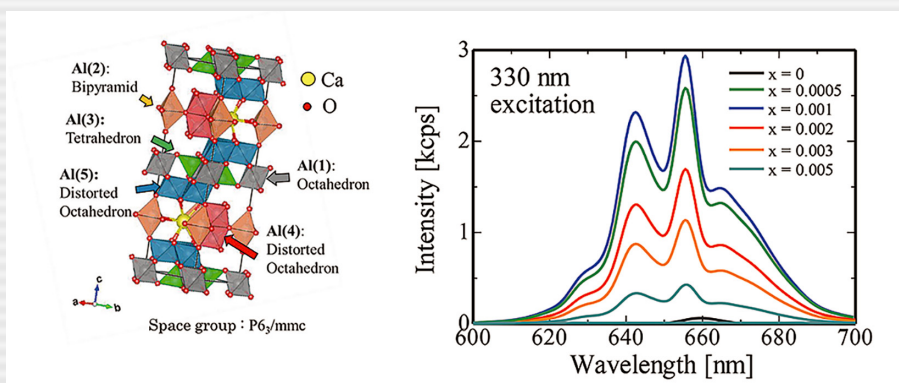
## ■代表論文および著書 / Representative publications

## 著書 / Book

1. 量子物質科学入門 量子化学と固体電子論：二つの見方（コロナ社）  
Introduction to quantum materials science (Corona Publishing Co. Ltd.)
2. 基礎材料科学（コロナ社）  
Fundamentals of Materials Science (Corona Publishing Co. Ltd.)

## 論文 / Paper

1. First-principles study of geometric and electronic structures, and optical transition energies of  $\text{Mn}^{4+}$  impurity ions:  $\text{K}_2\text{SiF}_6$  as a prototype, J. Lumin. 263 (2023) 120103
2. First-principles investigation of divalent ion sensing with cesium lead trihalides, Opt. Mater.: X 19 (2023) 10025
3. Geometrical and electronic structure analysis of Mn-doped  $\text{CaMO}_3$  ( $\text{M} = \text{Ti}, \text{Zr}$  and  $\text{Sn}$ ), Phys. Status Solidi B 260 (2023) 2200575
4. Support Vector Machine-Based Phase Prediction of Multi-principal Element Alloys, Vietnam J. Comp. Sci. 10 (2023) 101-106
5. Influence of co-doping of divalent ions on the photoluminescence intensity of  $\text{Mn}^{4+}$  doped  $\text{CaAl}_{12}\text{O}_{19}$ , Opt. Mater.: X 16 (2022) 100197
6. Theoretical and Experimental Investigations of  $\text{Mn}^{4+}$  Site Occupation in  $\text{CaAl}_{12}\text{O}_{19}$ , ECS J. Solid State Sci. Tech. 10 (2021) 076004
7. Evaluation of Damage Coefficient for Minority-Carrier Diffusion Length of Triple-Cation Perovskite Solar Cells under 1-MeV Electron Irradiation for Space Applications, J. Phys. Chem. C 125 (2021) 13131-13137
8. Unusual hydrogen implanted gold with lattice contraction at increased hydrogen content, Nature Comm. 12 (2021) 1560.
9. Evaluation of Damage Coefficient for Minority-Carrier Diffusion Length of Triple-Cation Perovskite Solar Cells under 1-MeV Electron Irradiation for Space Applications, J. Phys. Chem. C 125 (2021) 13131-13137.
10. Origin of room-temperature ferromagnetism in Co-doped  $\text{CeO}_2$ , Physica B 619 (2021) 413158.
11. Theoretical and Experimental Investigations of  $\text{Mn}^{4+}$  Site Occupation in  $\text{CaAl}_{12}\text{O}_{19}$ , ECS J. Solid State Sci. Tech. 10 (2021) 076004.
12. First-principles investigations of geometrical and electronic structures of  $\text{Mn}^{4+}$  doped  $\text{A}_2\text{SiF}_6$  ( $\text{A} = \text{K}, \text{Rb}, \text{Cs}$ ) red phosphors, Opt. Mat. 115 (2021) 110986.
13. Microstructure and diffusion behavior in the multilayered oxides formed on a Co-W electroplated ferritic stainless steel followed by oxidation treatment, Acta Materialia 194 (2020) 295-304



$\text{CaAl}_{12}\text{O}_{19}$ の結晶構造（左図）と $\text{CaAl}_{12(1-x)}\text{Mn}_{12x}\text{O}_{19}$ の蛍光スペクトル（右図）

Crystal structure of  $\text{CaAl}_{12}\text{O}_{19}$  (left) and observed photoluminescence spectra of  $\text{CaAl}_{12(1-x)}\text{Mn}_{12x}\text{O}_{19}$  (right).