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**COMPUTATIONAL STUDIES ON PHONON ENGINEERING OF  
TRANSITION METAL COMPOUNDS AND ITS INFORMATICS**

**Maezono, Ryo**  
**JAPAN ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY**  
**1-1, ASAHIDAI**  
**NOMI, ISHIKAWA, , 923-1211**  
**JP**

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## SECTION 2: TECHNICAL REPORT

# COMPUTATIONAL STUDIES ON PHONON ENGINEERING OF TRANSITION METAL COMPOUNDS AND ITS INFORMATICS

**PRINCIPAL INVESTIGATOR:** Associate Prof. Ryo Maezono

**AFFILIATION:** School of Information Science, Japan Advanced Institute of Science and Technology.

**ADDRESS:** Asahidai 1-1, Nomi, Ishikawa 923-1292, Japan.

**PHONE:** +81-761-51-1240

**EMAIL:** rmaezono@mac.com

**WEBPAGE:** <http://www.jaist.ac.jp/is/labs/maezono-lab/wiki/index.php>

## DISTRIBUTION STATEMENT

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## ABSTRACT

The 'phonon' means the quantum nature of lattice vibrations occurring in solids, being critically dominating thermoelectric, piezoelectric, photoelectric, and catalytic properties as well as the superconductivities. The reported project has worked on the cutting-edge of *ab initio* phonon estimations applied to the phonon engineering. It began with 2-dim. transition metal compounds, such as chalcogenides or pnictides to obtain comprehensive knowledge about phonon dispersions and those lattice instabilities. Since the simulation platform to carry out the project has made more progress than expected, the research activity has greatly been gone beyond the original narrow objectives targeting two-dimensional materials (target of application) and structural instability (target of analysis). The scope of application covers from 2,3-dimensional materials to polymers, and the scope of analysis covers from thermal conductivity to superconducting transition temperature. The development of informatics, which was only an item for future prospects at the time of the proposal, has made significant progress and now it is forming a part of our major research interests. As a result, the number of publications has increased significantly, from 39 to 99 during the term of the project (four years).

## 2.1; ACCOMPLISHMENTS

### 2.1.1; RESEARCH OBJECTIVES

The original objectives were the following three items. In addition to these, the human resource development described in §2.2.2 was also planned.

#### 2.1.1.1; SUPERLATTICE STRUCTURE AND PHONON PROPERTIES REALIZED IN LAYERED MATERIALS

We aimed at establishing the analytical procedure clarifying how the Peierls instability pronounced in low-dimensionality leads to the origin of the superlattice structure. It is performed by analyzing the appearance of imaginary modes coupled with the analysis of the shape of the Fermi surface. This was mainly planned in the first year of the project, and the results started to appear in 2017, which can be said to be a 100% completion rate.

#### 2.1.1.2; BROADER APPLICATIONS OF PHONON ANALYSIS

Estimated phonon frequencies are capable to be used as the input parameters for the model formulae of materials properties such as the superconducting transition temperature. It is useful

to predict the trend of the properties ranging among the materials. The subject is mainly planned for the second year of the project, with results coming in after 2020, which can be described as a 100% implementation rate.

### 2.1.1.3; DEVELOPMENT OF INFORMATICS BASED ON PHONON ANALYSIS

The trends obtained in the above can be described as regression relations and used for further informatics. This was mainly planned in the third year of the project, and the results are coming in after 2021. Four papers have been submitted, one of which is just about to be accepted soon (minor revision process). This is quite promising and ongoing in future, we can say that we have achieved 80%.

## 2.1.2; DETAILS OF ACCOMPLISHMENTS DURING THIS REPORTING PERIOD

### 2.1.2.1; SUPERLATTICE STRUCTURE AND PHONON PROPERTIES REALIZED IN LAYERED MATERIALS

As the theme most directly related to the grant proposal, we have developed research on phonon analysis of layered materials. The following papers have been published on these topics.

- \* A105; "Discovery of novel BCS-type superconductors in ThCr<sub>2</sub>Si<sub>2</sub>-type crystals via ab-initio and machine-learning techniques", G.S. Sinaga, K. Utimula, K. Nakano, K. Hongo, R. Maezono, <http://arxiv.org/abs/1911.10716>
- \* A89; "Synthesis, electronic structure and physical properties of layered oxypnictides Sr<sub>2</sub>ScCrAsO<sub>3</sub> and Ba<sub>3</sub>Sc<sub>2</sub>Cr<sub>2</sub>As<sub>2</sub>O<sub>5</sub>", S.P.K. Naik, Y. Iwasa, K. Kuramochi, Y. Ichihara, K. Kishio, K. Hongo, R. Maezono, T. Nishio, H. Ogino, **Inorg. Chem.** 60, 1930-1936 (2021/IF = 4.857/**Q1**).
- \* A83; "New layered perovskite family built from [CeTa<sub>2</sub>O<sub>7</sub>]-layers: coloring mechanism from the unique multi-transitions", T. Hasegawa, A. Shigee, Y. Nishiwaki, M. Nagasako, A.T. Hanindriyo, K. Hongo, R. Maezono, T. Ueda, Y. Asakura and S. Yin, **Chem Comm** 56, 8591 (2020/IF = 6.164/**Q1**)
- \* A59; "High pressure synthesis of A<sub>2</sub>NiO<sub>2</sub>Ag<sub>2</sub>Se<sub>2</sub> (A = Sr, Ba) with a high spin Ni<sup>2+</sup> in square planar coordination" (**Top 25%**), Y. Matsumoto, T. Yamamoto, K. Nakano, H. Takatsu, T. Murakami, K. Hongo, R. Maezono, H. Ogino, D. Song, C.M. Brown, C. Tassel, H. Kageyama, **Angew. Chem. Int. Ed.** 58, 756-759 (2019/IF = 11.709/**Q1**).
- \* A48; "Valence Band Engineering of Layered Bismuth Oxyhalides toward Stable Visible-Light Water Splitting: Madelung Site Potential Analysis" (**Top 5%**), D. Kato, K. Hongo, R. Maezono, M. Higashi, H. Kunioku, M. Yabuuchi, H. Suzuki, Z. Chengchao, K. Nakano, R. Abe, and H. Kageyama, **J. Am. Chem. Soc.** 139, 18725-18731 (2017/IF = 13.858/**Q1**).
- \* A47; "Investigation into structural phase transitions in layered titanium-oxypnictides by a computational phonon analysis", K. Nakano, K. Hongo, and R. Maezono, **Inorg. Chem.** 56, 13732-13740 (2017/IF = 4.857/**Q1**).

### 2.1.2.2; BROADER APPLICATIONS OF PHONON ANALYSIS

Not limited to the structural stability predictions, the phonon analysis can be applicable also to the estimations of phonon-based materials properties. Anharmonic effects are also the interesting application. The following papers have been published on these topics:

- \* A93; "Atomic forces by quantum Monte Carlo: Application to phonon dispersion calculations", K. Nakano, T. Morresi, M. Casula, R. Maezono, S. Sorella, **Phys. Rev. B** 103, L121110 (2021/IF = 3.736/**Q1**).
- \* A80; "Boron phosphide as a p-type transparent conductor: optical absorption and transport through electron-phonon coupling", V-A. Ha, B. Karasulu, R. Maezono, G. Brunin, J.B. Varley, G-M. Rignanese, B. Monserrat, and G. Hautier, **Phys. Rev. Mater.** 4, 065401 (2020/IF = 2.926/**Q1**)
- \* A78; "*Ab initio* thermodynamic properties of certain compounds in Nd-Fe-B system" (**Top25%**),

A.T. Hanindriyo, S. Sridar, K.C. Hari Kumar, K. Hongo, R. Maezono, **Comp. Mater. Sci.** 180, 109696 (2020/IF=2.644/**Q1**).

- \* A62; "First-principles anharmonic vibrational study of the structure of calcium silicate under lower mantle conditions", J.C.A. Prentice, R. Maezono, and R.J. Needs, **Phys. Rev. B** 99, 064101 (2019/IF = 3.836/**Q1**)

Based on the topic, we got a grant to invite an external researcher from India, staying a couple of months in my group:

- \* H33; "Computational study of electron/phonon transport in extremely scaled semiconductor devices", JSPS Invitation Fellowship Program for Research in Japan (Short Term) (Representative; 2018.5 - 2018.6; [150,000 JPY on top of the airfare and daily expenses (18,000JPY/day) to invite a researcher, Prof. Nihar Mohapatra [IIT Gandhinagar], staying in our group members for 1.5 months])

### **2.1.2.3; DEVELOPMENT OF INFORMATICS BASED ON PHONON ANALYSIS**

The following original papers have been published in the field of phonon analysis and its application to informatics such as machine learning.

- \* A115; "High- $T_c$  ternary metal hydride,  $YKH_{12}$  and  $LaKH_{12}$ , discovered by machine learning", P. Song, H. Zhufeng, P.B. de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono, <http://arxiv.org/abs/2103.00193>
- \* A112; "High  $T_c$  superconducting hydrides formed by the cage structures  $LaH_{24}$  and  $YH_{24}$  as basic blocks", P. Song, H. Zhufeng, P.B. de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono, <https://arxiv.org/abs/2107.05498>
- \* A111; "First-principles study on the phase diagram and superconductivity of Mg-Sc-H system under high pressure", P. Song, H. Zhufeng, P.B. de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono, <https://arxiv.org/abs/2109.07051>
- \* A109; "The systematic study on the stability and superconductivity of Y-Mg-H compounds under high pressure", P. Song, H. Zhufeng, P.B. de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono, <http://arxiv.org/abs/2103.00193>
- \* A68; "*Ab initio* search of polymer crystals with high thermal conductivity", K. Utimula, T. Ichibha, R. Maezono, K. Hongo, **Chem. Mater.** 13, 4649-4656 (2019/IF=10.159/**Q1**).

### **2.1.3; HOW WERE THE RESULTS DISSEMINATED TO COMMUNITIES OF INTEREST**

For the specialized community, we composed the following books:

- \* J10; Sec.'Theoretical calculations for mixed-anion compounds', R. Maezono, K. Hongo, A. Kuwahara, M. Ochi (Sec.5) in 'Science of mixed-anion compounds' (Maruzen/2021.3.30/ISBN : 978-4-621-30610-9).
- \* J09; Sec.'Wettability of surfaces analysed by *ab initio* modelling', K. Hongo, T. Muroto, R. Maezono (Sec.3.4) in 'Materials informatics; practical examples' (NTS/2021.1.20/ISBN : 978-4-86043-708-4).

In addition to talks at specialized societies, the following invited lectures and tutorials were given for audience from broader fields:

- \* B121; "Electronic structure calculation using Diffusion Monte Carlo methods", R. Maezono, 2021/04/28 (Invited/40 min.), 24rd International Annual Symposium on Computational Science and Engineering (ANSCSE24), April 28-30 2021, On-line.
- \* B120; 'How to estimate materials properties using *ab initio* simulation', Ryo Maezono, 2021/03/23 (Invited/30 min./online), Seminar on fundamental topics, annual meeting 2021, The Ceramic Society of Japan (CerSJ).
- \* B113; "How to setup computational environments for electronic structure calculations", R.

- Maezono, 2020/06/02 (Invited Lecture/120min./scheduled/postponed due to COVID19), 6th African School on Electronic Structure Methods and Applications (ASESMA-2020), 01-12 Jun. 2020, ICTP East African Institute for Fundamental Research, University of Rwanda, Kigali, Rwanda.
- \* B111; "Computational Approach to Material Design and Materials Informatics", R. Maezono, 2019/12/10 (Keynote/50 min. /scheduled), African Materials Research Society meeting, Arusha, Tanzania, 12/10-13, 2019.
  - \* B108; "Machine learning clustering technique applied to X-ray diffraction patterns to distinguish alloy substitutions", R. Maezono, 2019/06/27 (Invited/45 min.), 23rd International Annual Symposium on Computational Science and Engineering (ANSCSE23), June 27-29, Chiang Mai University, Chiang Mai, Thailand.
  - \* B107; "Machine learning clustering technique applied to X-ray diffraction patterns to distinguish alloy substitutions", R. Maezono, 2019/02/22 (Invited/45 min.), WOS AOARD/seminar on Computational Materials Science, Wright-Patterson AirForce Base, Dayton, Ohio, USA.
  - \* B104; "Computational phonon analysis applied to ThCr<sub>2</sub>Si<sub>2</sub>-type compounds", Aniwat Kesorn, K. Utimula, K. Hongo, R. Maezono, 2018/07/25 (invited /25 min.), 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications (CMCEE), Singapore.
  - \* B103; "High Performance Computing and Materials Simulations", R. Maezono, 2018/05/08 (invited /50 min.), Invited talk at NECTEC (National Institute of Electronics and Communication Technology), Bangkok, Thailand.
  - \* B102; "Recent progresses of Materials Informatics", R. Maezono, 2018/05/07 (invited /120 min.), Seminar talk at Faculty of Science (Physics and Chemistry), Mahidol Univ., Bangkok, Thailand.
  - \* B101; "Computational Approach to Material Design", R. Maezono, 2018/05/04 (keynote/50 min.), 3rd RSU National and International Research Conference on Science and Technology, Social Science, and Humanities 2018 (RSUSSH 2018), Rangsit Univ., Bangkok, Thailand.
  - \* B95; "Computational Approach to Material Design", R. Maezono, 2017/10/11 (keynote/40 min.), BICON-2017, Biyani College (Oct.11-13), Jaipur, India.

## 2.2; IMPACTS

### 2.2.1; FAMILIARIZING PHONON ANALYSIS AND HPC TO EXPERIMENTAL COMMUNITY

At the beginning of granted period, *ab initio* phonon analysis was still a tool for a limited theoretician's community. During the period, it became popular so rapidly among materials scientists that even experimentalists start to use it. Although *ab initio* static evaluations such as band alignment had been used even by experimentalists from the past, now the *ab initio* analysis gets expanded its range of applicability for practitioners with the idea of using phonon calculations on supercomputers to evaluate synthetic stability of their samples. Through the project, we developed many collaborations with synthetic experimentalists, achieving 21 co-authored papers (published/accepted) with 8 groups. Our group has accepted 11 visits of students from six institutions (Kyoto Univ., Kyushu Univ., AIST, Kyoto Univ., Tohoku Univ., Kanagawa Univ.) to teach *ab initio* technique running on supercomputers.

#### AIST

- \* A89; "Synthesis, electronic structure and physical properties of layered oxypnictides Sr<sub>2</sub>ScCrAsO<sub>3</sub> and Ba<sub>3</sub>Sc<sub>2</sub>Cr<sub>2</sub>As<sub>2</sub>O<sub>5</sub>", S.P.K. Naik, Y. Iwasa, K. Kuramochi, Y. Ichihara, K. Kishio, K. Hongo, R. Maezono, T. Nishio, H. Ogino, **Inorg. Chem.** 60, 1930-1936 (2021/IF = 4.857/**Q1**).

#### Tohoku University

- \* A73; "Chemical and structural stability of superconducting In<sub>5</sub>Bi<sub>3</sub> driven by relativistic spin-orbit coupling", S. Chen, R. Mae = NoStats/**Q1**).
- \* A88; "Intrinsic carbon-doping induced synthesis of oxygen vacancies-mediated TiO<sub>2</sub> nanocrystals: enhanced photocatalytic NO removal performance and mechanism" (**Top10%**), Z. Gu, Z. Cui, Z.

- Wang, K.S. Qin, Y. Asakura, T. Hasegawa, K. Hongo, R. Maezono, S. Yin, **J. Catal.** 393, 179-189 (2021/IF = 7.723/**Q1**)
- \* A87; "Carbon vacancies and hydroxyls in graphitic carbon nitride: promoted photocatalytic NO removal activity and mechanism" (**Top25%**), Z. Gu, Z. Cui, Z. Wang, K.S. Qin, Y. Asakura, T. Hasegawa, S. Tsukuda, K. Hongo, R. Maezono, S. Yin, **Applied Catalysis B: Environmental**, 279, 119376 (2020/IF=14.229/**Q1**)
- \* A86; "Octahedral morphology of NiO with (111) facet synthesized from the transformation of NiOHCl for NO<sub>x</sub> detection and degradation: Experiment and DFT calculation", A. Hermawan, A.T. Hanindriyo, E.R. Ramadhan, Y. Asakura, T. Hasegawa, K. Hongo, M. Inada, R. Maezono, and S. Yin, **Inorg. Chem. Front.** 7, 3431-3442 (2020/IF = 5.870/**Q1**).
- \* A83; "New layered perovskite family built from [CeTa<sub>2</sub>O<sub>7</sub>]-layers: coloring mechanism from the unique multi-transitions", T. Hasegawa, A. Shigee, Y. Nishiwaki, M. Nagasako, A.T. Hanindriyo, K. Hongo, R. Maezono, T. Ueda, Y. Asakura and S. Yin, **Chem Comm** 56, 8591 (2020/IF = 6.164/**Q1**)
- \* A63; "Synthesis of (Ba<sub>1-x</sub>Sr<sub>x</sub>)YSiO<sub>5</sub>N and Discussion based on Structure Analysis and DFT Calculation", T. Yasunaga, K. Hongo, K. Fujii, S. Yamamoto, R. Maezono, M. Yashima, M. Mitsuishi, H. Kato, M. Kobayashi, and M. Kakihana, **J. Solid State Chem.** 276, 266-271 (2019/IF = 2.179).

### Kyoto University

- \* A66; "Synthesis, optical properties, and band structures of a series of layered mixed-anion compounds", Y. Iwasa, H. Ogino, D. Song, V.C. Agulto, K. Yamanoi, T. Shimizu, J. Ueda, K. Hongo, R. Maezono, S. Tanabe, and N. Sarukura, **J. Mater. Sci.: Materials in Electronics** 30, 16827-16832 (2019/IF = 2.324/**Q1**).
- \* A60; "Crystal structure analysis and evidence of mixed anion coordination at the Ce<sup>3+</sup> site in Y<sub>3</sub>Al<sub>2</sub>(Al,Si)<sub>3</sub>(O,N)<sub>12</sub> oxynitride garnet phosphor" (**Top10%**), K. Asami, M. Shiraiwa, J. Ueda, K. Fujii, K. Hongo, R. Maezono, M. Brik, M. Yashima, S. Tanabe, **J. Mater. Chem. C** 7, 1330-1336 (2019/IF = 5.066/**Q1**).
- \* A59; "High pressure synthesis of A<sub>2</sub>NiO<sub>2</sub>Ag<sub>2</sub>Se<sub>2</sub> (A = Sr, Ba) with a high spin Ni<sup>2+</sup> in square planar coordination" (**Top 25%**), Y. Matsumoto, T. Yamamoto, K. Nakano, H. Takatsu, T. Murakami, K. Hongo, R. Maezono, H. Ogino, D. Song, C.M. Brown, C. Tassel, H. Kageyama, **Angew. Chem. Int. Ed.** 58, 756-759 (2019/IF = 11.709/**Q1**).
- \* A55; "Development of persistent phosphor of Eu<sup>2+</sup> doped Ba<sub>2</sub>SiO<sub>4</sub> by Er<sup>3+</sup> co-doping based on vacuum referred binding energy diagram" (**Top 25%**), K. Asami, J. Ueda, K. Yasuda, K. Hongo, R. Maezono, M.G. Brik, S. Tanabe, **Opt. Mater.** 84, 436-441 (2018/IF = 2.320/**Q1**)
- \* A48; "Valence Band Engineering of Layered Bismuth Oxyhalides toward Stable Visible-Light Water Splitting: Madelung Site Potential Analysis" (**Top 5%**), D. Kato, K. Hongo, R. Maezono, M. Higashi, H. Kunioku, M. Yabuuchi, H. Suzuki, Z. Chengchao, K. Nakano, R. Abe, and H. Kageyama, **J. Am. Chem. Soc.** 139, 18725-18731 (2017/IF = 13.858/**Q1**).

### Tokyo Institute of Technology

- \* A76; "Two-Dimensional Perovskite Oxynitride K<sub>2</sub>LaTa<sub>2</sub>O<sub>6</sub>N with an H<sup>+</sup>/K<sup>+</sup> Exchangeability in Aqueous Solution to Form Stable Photocatalyst for Visible-Light H<sub>2</sub> Evolution" (**Top10%**), T. Oshima, T. Ichibha, K. Oqmhula, K. Hibino, S. Yamashita, K. Fujii, Y. Miseki, K. Hongo, D. Lu, R. Maezono, K. Sayama, M. Yashima, K. Kimoto, H. Kato, M. Kakihana, H. Kageyama, K. Maeda, **Angew. Chem. Int. Ed.** 59, 2-10 (2020/IF = 11.709/**Q1**).
- \* A75; "Light Absorption Properties and Electronic Band Structures of Lead-Vanadium Oxyhalide Apatites Pb<sub>5</sub>(VO<sub>4</sub>)<sub>3</sub>X (X = F, Cl, Br, I)", M. Nakamura, K. Oqmhula, M. Eguchi, K. Oka, K. Hongo, R. Maezono, and K. Maeda, **Chem. Asian J.** 15, 540-545 (2020/IF = 3.698/**Q1**)
- \* A58; "Light Absorption Properties and Electronic Band Structures of Lead Titanium Oxyfluoride Photocatalysts Pb<sub>2</sub>Ti<sub>4</sub>O<sub>9</sub>F<sub>2</sub> and Pb<sub>2</sub>Ti<sub>2</sub>O<sub>5.4</sub>F<sub>1.2</sub>" (**Top 25%**), H. Wakayama, K. Utimura, T. Ichibha, R. Kuriki, K. Hongo, R. Maezono, K. Oka, and K. Maeda, **J. Phys. Chem. C** 122, 26506–26511 (2018/IF = 4.509/**Q1**).
- \* A53; "A Stable, Narrow-Gap Oxyfluoride Photocatalyst for Visible-Light Hydrogen Evolution and

- Carbon Dioxide Reduction" (**Top 1%**), R. Kuriki, T. Ichibha, K. Hongo, D. Lu, R. Maezono, H. Kageyama, O. Ishitani, K. Oka, and K. Maeda, **J. Am. Chem. Soc.** 140, 6648 (2018/IF = 13.858/**Q1**).
- \* A52; "Undoped Layered Perovskite Oxynitride  $\text{Li}_2\text{LaTa}_2\text{O}_6\text{N}$  for Photocatalytic  $\text{CO}_2$  Reduction with Visible-Light" (**Top 5%**), T. Oshima, T. Ichibha, K.S. Qin, K. Muraoka, J.J.M. Vequizo, K. Hibino, R. Kuriki, S. Yamashita, K. Hongo, T. Uchiyama, K. Fujii, D. Lu, R. Maezono, A. Yamakata, H. Kato, K. Kimoto, M. Yashima, Y. Uchimoto, M. Kakihana, O. Ishitani, H. Kageyama and K. Maeda, **Angew. Chem. Int. Ed.** 57, 8154-8158 (2018/IF = 11.709/**Q1**)

### Kyushu University

- \* A51; "Stabilization Mechanism of the Tetragonal Structure in a Hydrothermally Synthesized  $\text{BaTiO}_3$  Nanocrystal" (**Top 25%**), K. Hongo, S. Kurata, A. Jomphoak, M. Inada, K. Hayashi, R. Maezono, **Inorg. Chem.** 57, 5413-5419 (2018/IF = 4.857/**Q1**).

## 2.2.2; EDUCATIONAL ACTIVITIES FOR ASIAN AND AFRICAN SOCIETY THROUGH INTERNATIONAL TUTORIALS

As the outreach for utilizing supercomputer facilities in our institute, we have organized several international tutorial schools as follows to grow up international collaborative community.

### 2017

- \* International tutorial workshop (MEXT, electronic structure calculation), organized at JAIST, inviting four students and a faculty from IIT/Gandhinagar, one faculty from IIT/Madras.
- \* International tutorial workshop (MEXT, electronic structure calculation), organized at JAIST, inviting six students and two faculties from IIT/Gandhinagar, Delhi University, IISc.
- \* International tutorial workshop (JST, electronic structure calculation), organized at JAIST, inviting six students from India, Indonesia, Malesia, Thailand and Vietnam.
- \* Visiting Bandon Institute of Tech. (Indonesia) to introduce JAIST/MEXT oversea student scholarship.
- \* Visiting Vietnam National University Ho Chi Minh City to provide a lecture for dual degree program.

### 2018

- \* Visiting Ethiopia with a postgraduate student to give a lecture in 5th African School on Electronic Structure Methods and Applications (ASESMA-2018), organized by ICTP (International Centre for Theoretical Physics, UNESCO),
- \* Visiting IIT/Madras (India, Prof. Harikumar, Dept. of Metallurgy) taking a postgraduate student for the collaborative project.
- \* Visiting Chulalongkorn University (Thailand, Prof. Pornprasertsuk, Dept. of Materials Science), taking two postgraduate students to give a talk.

### 2019

- \* Visiting Chulalongkorn University (Thailand, Prof. Pornprasertsuk, Dept. of Materials Science), taking two postgraduate students to give a lecture course.
- \* International tutorial workshop (electronic structure calculation), organized at IIT/Madras, planned and organized by Maezono group.
- \* Workshop (electronic structure calculation) organized at JAIST, inviting two researchers from IIT/Madras.

### 2020

- \* Visiting IIT/Madras (India, Prof. Ravi Kumar, Dept. of Metallurgy) taking two postgraduate student for the collaborative project.
- \* Visiting Chulalongkorn University (Thailand, Prof. Bovornratanaraks, Dept. of Physics), taking two postgraduate students to give a lecture course (electronic structure calculation).

- \* Visiting Arusha International Conference Centre (Tanzania) to provide a tutorial (electronic structure calculation) in the workshop organized by ICTP (International Centre for Theoretical Physics, UNESCO), taking three postgraduate students.

## 2021

- \* Attending 6th African School on Electronic Structure Methods and Applications (ASESMA-2021, Web) to give a lecture, organized by ICTP (International Centre for Theoretical Physics, UNESCO),

With the partners from Asia and Africa, the following publications are achieved.

### India

- \* A96; "Surface study of  $\text{Cu}_2\text{SnS}_3$  using first-principles density functional theory", R. Dahule, A. Raghav, A.T. Hanindriyo, K. Hongo, R. Maezono, E. Panda, **Adv. Theory Simul.** 2000315 (2021/IF= 2.951/**Q1**)
- \* A94; "Insights into the mechanical and electrical properties of Metal-Phosphorene interface: An ab-initio study with a wide range of metals", A. Ghaffar, M.D. Ganeriwala, K. Hongo, R. Maezono, and N.R. Mohapatra, **ACS Omega** 6, 7795-7803 (2021/IF=2.580/**Q1**).
- \* A84; "Intrinsic Electronic Defect States of Anatase using Density Functional Theory", A. Raghav, A.T. Hanindriyo, K. Utimula, M. Abbasnejad, R. Maezono, E. Panda, **Comput. Mater. Sci.** 184, 109925 (2020/IF = 2.740/**Q1**)
- \* A78; "Ab initio thermodynamic properties of certain compounds in Nd-Fe-B system" (**Top25%**), A.T. Hanindriyo, S. Sridar, K.C. Hari Kumar, K. Hongo, R. Maezono, **Comp. Mater. Sci.** 180, 109696 (2020/IF=2.644/**Q1**).

### Indonesia

- \* A72; "A DFT+U Study of  $\text{H}_2\text{O}$  Molecule Adsorption and Dissociation on Stoichiometric and Non-Stoichiometric  $\text{CuO}(111)$  Surface" (**Top25%**), F. Ahmad, M.K. Agusta, R. Maezono, H. Dipojono, **J. Phys.: Condens. Matter**, 32, 045001 (2019/IF = 2.617/**Q1**).
- \* A64; "Density functional study of methyl butanoate adsorption and its C-O bonds cleavage on  $\text{MoS}_2$ -based catalyst with various Ni loads promoters", W.A.E. Prabowo, Subagio, Nugraha, M.K. Agusta, A.G. Saputro, S. Rustad, R. Maezono, W.A. Dino, H.K. Dipojono, **J. Phys. Condens. Matter** 31, 365001 (2019/IF = 2.617/**Q1**).
- \* A42; "Computational design of Ni-Zn based catalyst for direct hydrazine fuel cell catalyst using density functional theory" (**Top25%**), A.T. Hanindriyo, TB.M.Y.Y. Prawiraa, M.K. Agusta, R. Maezono, H.K. Dipojono. **Procedia Eng.** 170, 148-153 (2017) (IF = 0.73).
- \* A39; "Selectivity of CO and NO adsorption on  $\text{ZnO}(0002)$  surfaces: A DFT investigation" (**Top 10%**), Nugraha, A.G. Saputro, M.K. Agusta, B. Yulianto, H.K. Dipojono, F. Rusydi, and R. Maezono, **Applied Surface Science** 410, 373-382 (2017/IF = 3.150/**Q1**).

### Thailand

- \* A71; "3D structured Laser engraves decorated with gold nanoparticle SERS chips for herbicide detection in environments" (**Top5%**), R. Botta, P. Eiamchai, M. Horprathum, S. Limwichean, C. Chananonawathorn, V. Patthanasettakul, R. Maezono, A. Jomphoak and N. Nuntawong, **Sensors and Actuators B: Chemical**, 304, 127327 (2019/IF = 6.393/**Q1**).
- \* A54; "Host-Guest Interactions of Plumbagin with  $\beta$ -Cyclodextrin, Dimethyl- $\beta$ -Cyclodextrin and Hydroxypropyl- $\beta$ -Cyclodextrin: Semi-Empirical Quantum Mechanical PM6 and PM7 Methods" (**Top25%**), O. Srihakulung, R. Maezono, P. Toochinda, W. Kongprawechnon, A. Intarapanich, L. Lawtrakul, **Sci. Pharm.** 86, 20:1-11 (2018/IF = 1.64).
- \* A49; "Density Functional Theory Simulations of Aluminium Alkoxide and Fluoride", A. Jomphoak, T. Onjun, K. Hongo, R. Maezono, **Int. J. New Tech. Res. (IJNTR)** 3, 12-14 (2017/IF = 2.254).

### Kenya

- \* A50; "Adhesion of Electrodes on Diamond (111) Surface: A DFT Study", T. Ichibha, K. Hongo, I. Motochi, N.W. Makau, G.O. Amolo, R. Maezono, **Diam. Relat. Mater.** 81, 168-175 (2018/IF =

2.561/Q1)

### Cameroon

- \* A44; "Influence of endohedral confinement of atoms on structural and dynamical properties of the C60 fullerene", A.J. Etindele, R. Maezono, R.L.M. Melono, and O. Motapon, **Chemical Physics Letters** 685C, 395-400 (2017) (IF = 1.815).

In addition to Asian/African countries, the following international collaborations have achieved publications.

### UK/Cambridge, Lancaster

- \* A73; "Chemical and structural stability of superconducting  $\text{In}_5\text{Bi}_3$  driven by relativistic spin-orbit coupling", S. Chen, R. Maezono, J. Chen, F.M. Grosche, C.J. Pickard, and B. Monserrat, **J. Phys. Mater.** 3, 015007 (2019/IF= NoStats/Q1).
- \* A62; "First-principles anharmonic vibrational study of the structure of calcium silicate under lower mantle conditions", J.C.A. Prentice, R. Maezono, and R.J. Needs, **Phys. Rev. B** 99, 064101 (2019/IF = 3.836/Q1)
- \* A56; "Quantum Monte Carlo calculations of energy gaps from first principles" (**Top10%**), R.J. Hunt, M. Szyniszewski, G.I. Prayogo, R. Maezono, N.D. Drummond, **Phys. Rev. B** 98, 075122 (2018/IF = 3.836/Q1)
- \* A45; "Diffusion quantum Monte Carlo study of excitonic complexes in two-dimensional transition-metal dichalcogenides" (**Top 5%**), E. Mostaani, M. Szyniszewski, C.H. Price, R. Maezono, M. Danovich, N.D. Drummond, and V.I. Fal'ko, **Phys. Rev. B** 96, 075431 (2017) (IF = 3.836/Q1).
- \* A41; "Quantum Monte Carlo study of the energetics of rutile, anatase, brookite and columbite  $\text{TiO}_2$  polymorphs" (**Top10%**), J. Trail, B. Monserrat, P.L. Rios, R. Maezono, and R.J. Needs, **Phys. Rev. B** 95, 121108(R) (2017). (IF = 5.1/Q1)

### Italy/SISSA

- \* A77; "Speeding up the *ab initio* diffusion Monte Carlo by a smart lattice regularization" (**Top25%**), K. Nakano, R. Maezono, S. Sorella, **Phys. Rev. B** 101, 155106 (2020/IF = 3.836/Q1).
- \* A67; "All-electron quantum Monte Carlo with Jastrow single determinant Ansatz: application to the sodium dimer" (**Top25%**), K. Nakano, R. Maezono, and S. Sorella, **J. Chem. Theory Comput.** 15, 4044-4055 (2019/IF = 5.39/Q1).

### US/Oakridge

- \* A104; "Making the most of data: Quantum Monte Carlo Post-Analysis Revisited", T. Ichibha, K. Hongo, R. Maezono, A.J.W. Thom, <http://arxiv.org/abs/1904.09934>
- \* A101; "New structure *Pbam*-8 giving competitive stability at higher pressure range of dense hydrogen", T. Ichibha, Y. Zhang, K. Hongo, F. Reberdo, and R. Maezono, under review (**Phys. Rev. B**/IF = 3.736).

### US/Argonne

- \* A99; "Importance of van der Waals interaction in hydrogen adsorption on silicon-carbide nanotube revisited with vdW-DFT and QMC", G.I. Prayogo, H. Shin, A. Benali, R. Maezono, K. Hongo, **ACS Omega** 6, 24630-24636 (2021) (2021/IF=2.580/Q1).
- \* A70; "Ti interstitial flows giving rutile  $\text{TiO}_2$  reoxidation process enhanced in (001) surface", T. Ichibha, A. Benali, K. Hongo, and R. Maezono, **Phys. Rev. Mater.** 3, 125801 (2019/IF = 3.337/Q1).

### US/Airforce

- \* A108; "Reinforcement learning autonomously identifying the source of errors for agents in a group mission", K. Utimula, K. Hayaschi, K. Nakano, K. Hongo and R. Maezono, <http://arxiv.org/abs/2107.09232>

## 2.2.3; TEXTBOOKS AND COURSE DESIGNS

Two books on topics related to the present project was composed and published. For J08, English translated version is under preparation, planed to be published from Springer-Nature Publishing Co., Ltd. soon.

\*J07; 'Most comprehensive introduction how to construct PC cluster'  
(自作 PC クラスタ超入門--ゼロからはじめる並列計算環境の構築と運用), Ryo Maezono,  
Morikita Publishing Co., Ltd. (176pages, 2017/12/14), ISBN-13: 978-4627818217

\*J08; 'Hand-on tutorial of *ab initio* electronic structure calculation'  
(動かして理解する第一原理電子状態計算), Ryo Maezono and Tom Ichibha,  
Morikita Publishing Co., Ltd. (208pages, 2020/9/19), ISBN-13: 978-4627170315

During the period, several teaching courses have also been established at University on Quantum annealing, Quantum Materials Informatics, and Statistical signal processing (lecture notes are openly available from group web page).

## 2.2.4; OTHER TOPICS

Although not directly related to the present theme, the project has stimulated updated interest in the following topics, producing recent publications.

### 2.2.4.1; INFORMATICS

- \* A108; "Reinforcement learning autonomously identifying the source of errors for agents in a group mission", K. Utimula, K. Hayaschi, K. Nakano, K. Hongo and R. Maezono, <http://arxiv.org/abs/2107.09232>
- \* A106; "Feature space of XRD patterns constructed by auto-encoder", K. Utimula, M. Yano, H. Kimoto, K. Hongo, K. Nakano and R. Maezono, <https://arxiv.org/abs/2005.11660>
- \* A95; "A Quantum annealing approach to Ionic Diffusion in Solids", K. Utimula, T. Ichibha, G. Prayogo, K. Hongo, K. Nakano and R. Maezono, **Sci. Rep.** 11, 7261 (2021/IF = 5.228/**Q1**)
- \* A92; "Exploring Heat-Shielding Nanoparticle-Based Materials Via First-Principles Calculations and Transfer Learning", T. Yoshida, R. Maezono, K. Hongo, **ACS Appl. Nano Mater.** 4, 1932 (2021/**Q1**)
- \* A91; "Stochastic estimations of the total number of classes for a clustering having extremely large samples to be included in the clustering engine", K. Utimula, K. Nakano, K. Hongo, and R. Maezono, **Adv. Theory Simul.** 2000301 (2021/IF= 2.951/**Q1**)
- \* A40; "Bayesian Molecular Design with A Chemical Language Model" (**Top 5%**), H. Ikebata, K. Hongo, T. Isomura, R. Maezono, and R. Yoshida, **J. Comput. Aided Mol. Des.** 31, 379 (2017/IF = 3.199).

### 2.2.4.2; AB INITIO QUANTUM MONTE CARLO

- \* A104; "Making the most of data: Quantum Monte Carlo Post-Analysis Revisited", T. Ichibha, K. Hongo, R. Maezono, A.J.W. Thom, <http://arxiv.org/abs/1904.09934>
- \* A103; "Diffusion Monte Carlo evaluation of disiloxane linearization barrier", A.T. Hanindriyo, A.K.S. Yadav, T. Ichibha, R. Maezono, K. Nakano, and K. Hongo, **arXiv**:2010.06767
- \* A101; "New structure *Pbam*-8 giving competitive stability at higher pressure range of dense hydrogen", T. Ichibha, Y. Zhang, K. Hongo, F. Reboredo, and R. Maezono, under review (Phys. Rev. B/IF = 3.736).
- \* A90; "GaN band-gap bias caused by semi-core treatment in pseudopotentials analyzed by the diffusion Monte Carlo method", Y. Nikaido, T. Ichibha, K. Nakano, K. Hongo, and R. Maezono, **AIP Adv.** 11, 025225 (2021/IF = 1.579).
- \* A85; "*Ab initio* evaluation of complexation energies for cyclodextrin drug-inclusion complexes", K. Oqmhula, K. Hongo, R. Maezono\* and T. Ichibha, **ACS Omega** 5, 19371 (2020/IF=2.580/**Q1**).
- \* A77; "Speeding up the *ab initio* diffusion Monte Carlo by a smart lattice regularization" (**Top25%**), K. Nakano, R. Maezono, S. Sorella, **Phys. Rev. B** 101, 155106 (2020/IF = 3.836/**Q1**).

- \* A74; "Inconsistencies in *ab initio* evaluations of non-additive contributions of DNA stacking energies" (**Top25%**), K.S. Qin, T. Ichibha, K. Hongo, and R. Maezono, **Chem. Phys.** 529, 110554 (2020/IF = 1.707).
- \* A70; "Ti interstitial flows giving rutile TiO<sub>2</sub> reoxidation process enhanced in (001) surface", T. Ichibha, A. Benali, K. Hongo, and R. Maezono, **Phys. Rev. Mater.** 3, 125801 (2019/IF = 3.337/**Q1**).
- \* A67; "All-electron quantum Monte Carlo with Jastrow single determinant Ansatz: application to the sodium dimer" (**Top25%**), K. Nakano, R. Maezono, and S. Sorella, **J. Chem. Theory Comput.** 15, 4044-4055 (2019/IF = 5.39/**Q1**).
- \* A56; "Quantum Monte Carlo calculations of energy gaps from first principles" (**Top10%**), R.J. Hunt, M. Szyniszewski, G.I. Prayogo, R. Maezono, N.D. Drummond, **Phys. Rev. B** 98, 075122 (2018/IF = 3.836/**Q1**).
- \* A45; "Diffusion quantum Monte Carlo study of excitonic complexes in two-dimensional transition-metal dichalcogenides" (**Top 5%**), E. Mostaani, M. Szyniszewski, C.H. Price, R. Maezono, M. Danovich, N.D. Drummond, and V.I. Fal'ko, **Phys. Rev. B** 96, 075431 (2017) (IF = 3.836/**Q1**).
- \* A43; "New Insight into the Ground State of FePc: A Diffusion Monte Carlo Study", T. Ichibha, Z. Hou, K. Hongo, and R. Maezono, **Sci. Rep.** 7, 2011 (2017) (IF = 5.228/**Q1**).
- \* A41; "Quantum Monte Carlo study of the energetics of rutile, anatase, brookite and columbite TiO<sub>2</sub> polymorphs" (**Top10%**), J. Trail, B. Monserrat, P.L. Rios, R. Maezono, and R.J. Needs, **Phys. Rev. B** 95, 121108(R) (2017). (IF = 5.1/**Q1**)

#### **2.2.4.3; OTHER PROPERTIES OF MATERIALS**

- \* A100; "Interface modelling for *ab initio* evaluation of contact angle on a metallic surface", T. Murono, K. Hongo, K. Nakano, R. Maezono, <http://arxiv.org/abs/2009.11497>
- \* A70; "Ti interstitial flows giving rutile TiO<sub>2</sub> reoxidation process enhanced in (001) surface", T. Ichibha, A. Benali, K. Hongo, and R. Maezono, **Phys. Rev. Mater.** 3, 125801 (2019/IF = 3.337/**Q1**).
- \* A69; "Method for the Calculation of the Hamaker constants of Organic Materials by the Lifshitz Macroscopic Approach With DFT", H. Takagishi, T. Masuda, T. Shimoda, R. Maezono, and K. Hongo, **J. Phys. Chem. A** 123, 8726-8733 (2019/IF = 2.836/**Q1**).
- \* A46; "A computational scheme to evaluate Hamaker constants of molecules with practical size and anisotropy", K. Hongo and R. Maezono, **J. Chem. Theory Comput.** 13, 5217 (2017). (IF = 5.39/**Q1**).
- \* A61; "A new *ab initio* modeling scheme for the ion self-diffusion coefficient applied to the  $\epsilon$ -Cu<sub>3</sub>Sn phase of the Cu-Sn alloy", T. Ichibha, G. Prayogo, K. Hongo, R. Maezono, **Phys. Chem. Chem. Phys.** 21, 5158-5164 (2019/IF = 4.493/**Q1**).

#### **2.2.5; COLLABORATIVE APPLICATIONS FOR GRANTS**

As a centripetal force for collaboration, joint grant applications are quite effective. Through this project, we have constructed tighter partnership for cooperative applications.

##### **[Domestic/experimental group]**

- \* JST-CREST(2018/2019/2021a/2021b; unsuccessful)
- \* MEXT-KAKENHI(2019/2020; unsuccessful)
- \* MEXT-KAKENHI(2021; submitted)

##### **[International]**

- \* MEXT-Fostering Joint International Research (UK/with Lancaster University/2018; successful)
- \* JSPS Invitation Fellowship (India/with IIT Gandhinagar/2018; successful)
- \* JSPS Bilateral Joint Projects (India/with IIT Madras/2019; successful)
- \* JSPS Bilateral Joint Projects (Thai/with IIT Madras/2021; submitted)

#### **2.2.6; COLLABORATIONS WITH INDUSTRIAL DOMAIN**

The activity has also developed industry-academia collaboration on phonon analysis and informatics.

achieving the following co-authored publications.

### [Sumitomo Mining]

- \* A97; "High-throughput evaluation of discharge profiles in  $\text{LiNi}_{1-x}\text{X}_x\text{O}_2$  by *ab initio* calculations", S. Yoshio, K. Hongo, K. Nakano, and R. Maezono, **J. Phys. Chem. C** **125**, 14517-14524 (2021, IF = 4.772/**Q1**)
- \* A92; "Exploring Heat-Shielding Nanoparticle-Based Materials Via First-Principles Calculations and Transfer Learning", T. Yoshida, R. Maezono, and K. Hongo, **ACS Appl. Nano Mater.** **4**, 1932-1939 (2021/**Q1**)
- \* A82; "Synergy of Binary Substitution for Improving Cycle Performance in  $\text{LiNiO}_2$  Revealed by *ab Initio* Materials Informatics", T. Yoshida, R. Maezono, and K. Hongo, **ACS Omega** **5**, 13403-13408 (2020/IF= 2.580/**Q1**).
- \* A79; "Electrochemical Properties and Crystal Structure of  $\text{Li}^+/\text{H}^+$  Cation-exchanged  $\text{LiNiO}_2$ " (**Top10%**) T. Toma, R. Maezono, K. Hongo, **ACS Appl. Energy Mater.** **4**, 4078-4087 (2020/IF= NoStats (new journal)/**Q1**).
- \* A65; "First-Principles Study of Structural Transition in  $\text{LiNiO}_2$  and High Throughput Screening for Long Life Battery" (**Top25%**), T. Yoshida, K. Hongo, and R. Maezono, **J. Phys. Chem. C** **123**, 14126-14131 (2019/IF = 4.509/**Q1**).

### [Toyota Motor]

- \* A81; "Machine learning clustering technique applied to powder X-ray diffraction patterns to distinguish compositions of  $\text{ThMn}_{12}$ -type alloys", K. Utimula, R. Hunkao, M. Yano, H. Kimoto, K. Hongo, S. Kawaguchi, S. Suwana, R. Maezono, **Adv. Theory Simul.** **3**, 2000039:1-9 (2020/IF= NoStats (new journal)/**Q1**).
- \* A106; "Feature space of XRD patterns constructed by auto-encoder", K. Utimula, M. Yano, H. Kimoto, K. Hongo, K. Nakano and R. Maezono, <https://arxiv.org/abs/2005.11660>

## 2.2.7; OUTREACH ACTIVITIES

Activities have been undergone for the publicity disseminating that quantum mechanical simulations are useful for environment and energy via materials development.

The book J07 (in Sec.2.2.3) worked well in this aspect because the primary readership is non-expert of the topic. The following general lectures also serve this purpose.

- \* B118; "Experience in the collaborative education on simulations", Ryo Maezono, 2021/01/07 (Invited/90 min.), 34th-round CAMM forum, Business Research Institute, Aoyama, Tokyo.
- \* B117; "Handmade PC cluster utilized in materials simulations", Ryo Maezono, 2020/12/05 (Keynote/60 min.), Open CAE, Front ISTR joint symposium 2020, online.