## 業績リスト

#### 深澤 太郎

#### 2018年11月19日

## 査読付き論文

- T. Fukazawa and H. Akai. A new practical scheme for the optimized effective potential method. Journal of Physics: Condensed Matter, Vol. 22, p. 405501, 2010.
- S. Iwasaki, T. Fukazawa, M. Ogura, and H. Akai. First-principles calculations of YMn<sub>2</sub>. *Journal of the Physical Society of Japan Supplement*, Vol. 81, p. SB032, 2012.
- Masaaki Geshi and Taro Fukazawa. Pressure induced band gap opening of AlH<sub>3</sub>. Physica B: Condensed Matter, Vol. 411, p. 154, 2012.
- Taro Fukazawa, Akihisa Kiyota, and Chuzo Ninagawa. Aggregated transfer function for smart grid FastADR feedback control of wide area distributed building facilities. *IEEJ Transactions on Electrical* and Electronic Engineering, Vol. 10, No. 4, p. 487, 2015.
- Taro Fukazawa and Hisazumi Akai. Optimized effective potential method and application to static RPA correlation. Journal of Physics: Condensed Matter, Vol. 27, No. 11, p. 115502, 2015.
- Taro Fukazawa, Tomohisa Yamada, and Chuzo Ninagawa. Theoretical performance analysis on trasmission reserve table buffer with triage ranking for resource-limited control networks. *IEEJ Trans*actions on Electrical and Electronic Engineering, Vol. 11, No. 1, p. 91, 2016.
- Taro Fukazawa, Yuji Iwata, Junji Morikawa, and Chuzo Ninagawa. Stabilization of neural network
  by combination with ar model in FastADR control of building air-conditioner facilities. *IEEJ Trans-*actions on Electrical and Electronic Engineering, Vol. 11, No. 1, p. 124, 2016.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles study of intersite magnetic couplings in NdFe<sub>12</sub> and NdFe<sub>12</sub>X (X = B, C, N, O, F). *Journal of Applied Physics*, Vol. 122, No. 5, p. 053901, 2017.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles Study of Intersite Magnetic Couplings and Curie Temperature in RFe<sub>12-x</sub>Cr<sub>x</sub> (R= Y, Nd, Sm). Journal of Physical Society of Japan, Vol. 87, No. 4, 2018.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles study of spin-wave dispersion in Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>12</sub>. Journal of Magnetism and Magnetic Materials, Vol. 469, pp. 296 – 301, 2019.
- Yosuke Harashima, Taro Fukazawa, Hiori Kino, and Takashi Miyake. Effect of R-site substitution and the pressure on stability of RFe<sub>12</sub>: A first-principles study. Journal of Applied Physics, Vol. 124,

### 国際会議における発表

- T. Fukazawa and H. Akai. Exact-exchange based investigation of heusler alloys. In *The 10th Asian Workshop on First-principles electronic Structure Calculations*, Hiroshima University, Higashi-Hiroshima, Japan, October 2007. Poster presentation.
- T. Fukazawa and H. Akai. An effective approximate method of determining optimized effective potentials for extended systems. In *International Conference on Quantum Simulators and Design 2008*, Tokyo, Japan, May 2008. Poster presentation.
- Taro Fukazawa and Hisazumi Akai. A fast optimized effective potential method with EXX and RPA level correlation. In *International Symposium of Electronic Structure Calculations Theory, Correlated and Large Scale Systems and Numerical methods*–, University of Tokyo, Japan, December 2009. Poster presentation.
- Taro Fukazawa and Hisazumi Akai. Development of a method of first principles electronic structure calculation using optimized effective potential. In 3rd-ICNDR: International Conference of Core Research and Engineering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization, May 2010. Poster presentation.
- Taro Fukazawa and Hisazumi Akai. Practical method of OEP scheme and its application to rpa level correlation energy. In Psi-k Conference 2010, Henry Ford Building, Berlin, Germany, September 2010.
   Oral presentation.
- Taro Fukazawa. Development of a method of first-principles electronic structure calculation using the optimized effective potential method. In *INSD Nanoscience Seminar (No.2)*, Graduate School of Science, Osaka University, Japan, February 2011. Oral presentation.
- Taro Fukazawa. Development of a method of first-principles calculation using the optimized effective potentials. In "International Workshop on Nano-Spintronics" and "JSPS core-to-Core Program Kick-Off Meeting", June 2012. Poster presentation.
- Taro Fukazawa. Reformulated optimized effective potentials and its application with static random-phase-approximation correlation. In *International Symposium on Computics: Quantum Simulation and Design (ISC-QSD)*, Osaka University Hall, Osaka, Japan, October 2012. Poster presentation.
- Takao Kotani, Hiori Kino, and Taro Fukazawa. Quasiparticle self-consistent gw method in the linearlized (apw+mto) method. In *International Symposium on Computics: Quantum Simulation and Design (ISC-QSD)*, Osaka University Hall, Osaka, Japan, October 2012. Poster presentation.
- Masaaki Geshi and Taro Fukazawa. Band gap opening of AlH<sub>3</sub> under high pressure. In 8th Handai Nanoscience and Nanotechnology International Symposium, Icho-kaikan, Osaka University, Japan, December 2012. Poster presentation.
- Taro Fukazawa and Hisazumi Akai. Optimized effective potential method and its application to static RPA correlation. In *Green's Functions in ab initio Electronic Structure Calculations of Solids:* From Implementation to Applications, Physikzentrum Bad Honnef, Germany, February 2015. Oral

- presentation.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. Inter-site magnetic couplings in NdFe<sub>12- $\delta$ </sub>M $_{\delta}$  (M = K-Br). In *CSW2017*, Shonan Village Center, Japan, March 2017. Poster presentation.
- Yosuke Harashima, Taro Fukazawa, Kiyoyuki Terakura, Hiori Kino, Shoji Ishibashi, and Takashi Miyake. Effects of crystal structure and nitrogenation on magnetization and magnetocrystalline anisotropy in  $Y_{n-m}Fe_{5n+2m}$  [(n,m)=(1,0), (2,1), (3,1)]. In CSW2017, Shonan Village Center, Japan, March 2017. Poster presentation.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles study of spinwave dispersion in Sm(FeCo)<sub>12</sub>. In *Intermag2018*, Marina Bay Sands Convention Centre, Singapore, April 2018. Poster presentation.
- Zhufeng Hou, Taro Fukazawa, Yosuke Harashima, Kiyoyuki Terakura, and Takashi Miyake. First-principles study on stability and magnetism of ZFe<sub>12</sub> (Z from K to Rn) compounds. In *The 25th International Conference on Rare-Earth Permanent Magnets and Their Applications (REPM2018)*, Peking University, China, August 2018. Oral presentation.

## 国内の会議における発表

- 深澤太郎,赤井久純. 最適化有効ポテンシャル法を用いた第一原理電子状態計算手法. 日本物理学会第63回年次大会, Kinki University, Osaka, Japan, March 2008. Oral presentation.
- 岩崎将, 深澤太郎, 赤井久純. Y<sub>1-x</sub>Lu<sub>x</sub>Mn<sub>2</sub>(x=0~0.05) の電子状態と磁性. 日本物理学会第 64 回年次大会, Rikkyo University, Tokyo, Japan, March 2009. Oral presentation.
- 深澤太郎,赤井久純. 最適化有効ポテンシャル法を用いた第一原理電子状態計算における相関項の計算手法.
   日本物理学会 2009 年秋季大会, Kumamoto University, Japan, September 2009. Oral presentation.
- 深澤太郎, 岩崎将, 赤井久純. KKR-Green 関数法を用いたヘリカル磁性体 YMn<sub>2</sub> の電子状態計算. 日本物理学会 2009 年秋季大会, Kumamoto University, Japan, September 2009. Oral presentation.
- 岩崎将,深澤太郎,赤井久純. YMn<sub>2</sub> および Y<sub>1-x</sub>Lu<sub>x</sub>Mn<sub>2</sub> の磁性. 日本物理学会 2009 年秋季大会, Kumamoto University, Japan, September 2009. Oral presentation.
- 深澤太郎,赤井久純. 最適化有効ポテンシャル法を用いた第一原理電子状態計算. 日本物理学会第 65 回年次大会, Okayama University, Japan, March 2010. Oral presentation.
- 下司雅章, 深澤太郎. AlH<sub>3</sub> の圧力誘起金属-半導体転移. 日本物理学会第 68 回年次大会, Hiroshima University, Japan, March 2013. Oral presentation.
- 深澤太郎,赤井久純,原嶋庸介,三宅隆. 磁石化合物 Nd(Fe<sub>12-x</sub>M<sub>x</sub>)X (M=Ti, Co; X= B, C, N, O, F) におけるサイト間磁気結合の第一原理電子状態計算. 日本物理学会第 71 回年次大会, Tohoku Gakuin University, Japan, March 2016. Poster presentation.
- 深澤太郎, 赤井久純, 原嶋庸介, 三宅隆. 第一原理電子状態計算に基づく NdFe<sub>12</sub> および NdFe<sub>12</sub>X (X = B, C, N, O, F) のサイト間磁気結合の研究. 第 1 回ポスト「京」重点課題 (7) 研究会, The University of Tokyo, Japan, July 2016. Poster presentation.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles study of

- inter-site magnetic couplings in NdFe<sub>12</sub> and NdFe<sub>12</sub>X (X = B, C, N, O, F). TIA "かけはし" ポスター 交流会, EPOCHAL TSUKUBA, Japan, August 2016. Poster presentation.
- 深澤太郎,赤井久純,原嶋庸介,三宅隆.磁石化合物 Nd(Fe<sub>12-δ</sub>M<sub>δ</sub>)(M=K-Br) のサイト間磁気結合の第一原理電子状態計算. 日本物理学会第 72 回年次大会, pp. 1199-1199, Osaka University, Japan, March 2017. Oral presentation.
- 深澤太郎, 赤井久純, 原嶋庸介, 三宅隆. コヒーレントポテンシャル近似を用いた DFT 計算に基づく磁石 化合物の NdFe<sub>12-x</sub>M<sub>x</sub> (M = K−Br) のキュリー温度計算. 第 2 回ポスト「京」重点課題 (7) 研究会, The University of Tokyo, Japan, July 2017. Poster presentation.
- 原嶋庸介, 深澤太郎, 寺倉清之, 木野日織, 石橋章司, 三宅隆. RFe<sub>12</sub> の安定性に対する希土類元素置換効果の第一原理的研究. 第2回ポスト「京」重点課題 (7) 研究会, The University of Tokyo, Japan, July 2017. Poster presentation.
- 深澤太郎. First-principles investigation of the curie temperature in NdFe<sub>12-x</sub>M<sub>x</sub> (M=K-Br). 元素 戦略磁性材料研究拠点成果公開シンポジウム, TKP ガーデンシティ PREMIUM 名駅西口, Japan, June 2017. Poster presentation.
- 深澤太郎, 赤井久純, 原嶋庸介, 三宅隆. 磁石化合物 RFe<sub>12-x</sub>Cr<sub>x</sub>(R=Y, Nd, Sm)におけるサイト間磁気結合の第一原理電子状態計算. 日本物理学会 2017 年秋季大会, Iwate University, Japan, September 2017. Oral presentation.
- 原嶋庸介,深澤太郎,寺倉清之,木野日織,石橋章司,三宅隆. YFe<sub>12</sub>N および Y<sub>2</sub>Fe<sub>17</sub>N<sub>3</sub> の磁性における窒素の効果と結晶構造との関係に対する第一原理的研究. 日本物理学会 2017 年秋季大会, Iwate University, Japan, September 2017. Oral presentation.
- Taro Fukazawa. First-principles based calculation of the curie temperature for magnetic compounds NdFe<sub>12-x</sub>M<sub>x</sub> (M=K--Br). TIA "かけはし" ポスター交流会, The University of Tokyo, Japan, September 2017. Poster presentation.
- 深澤太郎, 赤井久純, 原嶋庸介, 三宅隆. 第一原理計算に基づく磁石化合物 RFe<sub>12-x</sub>Cr<sub>x</sub> (R=Y, Nd, Sm) のサイト間磁気結合. PCoMS シンポジウム&計算物質科学スパコン共用事業報告会 2017, Tohoku University, Japan, November 2017. Poster presentation.
- 深澤太郎, 原嶋庸介, 三宅隆. Search for magnet compounds using bayesian optimization. NIMS 学術シンポジウム「磁性材料イノベーション」, Tokyo International Forum, October 2018. Poster presentation.
- 深澤太郎. ベイズ最適化と第一原理電子状態計算を用いた磁石化合物の探索. PCoMS シンポジウム&計算物質科学スパコン共用事業報告会 2018, Tohoku University, Japan, October 2018. Oral presentation.
- 原嶋庸介,深澤太郎,木野日織,三宅隆.ベイズ最適化と第一原理電子状態計算を用いた磁石化合物の探索. PCoMS シンポジウム&計算物質科学スパコン共用事業報告会 2018, Tohoku University, Japan, October 2018. Oral presentation.
- 深澤太郎. 第一原理計算と情報統合型手法による新磁石化合物の探索. 第 5 回成果報告会第 5 回「京」を中核とする HPCI システム利用研究課題成果報告会, THE GRAND HALL, Shinagawa, Japan, November 2018. Poster presentation.

# 賞罰

- Student poster award, June 2010. 3rd-ICNDR: International Conference of Core Research and Enginnering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization.
- Best RA award, 2011. "Core Research and Engineering of Advanced Materials—Interdisciplinary Education Center for Materials Science" project, Osaka University, supported by Global COE program, MEXT, Japan.
- A winner of "Art in magnetism" contest by Judges' Selection, 2011. 2018 IEEE International Magnetics Conference (Intermag2018).