

# 業績リスト

深澤 太郎

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## 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, September 2010.
- S. Iwasaki, T. Fukazawa, M. Ogura, and H. Akai. First-principles calculations of  $\text{YMn}_2$ . *Journal of the Physical Society of Japan Supplement*, Vol. 81, p. SB032, November 2012.
- Masaaki Geshi and Taro Fukazawa. Pressure induced band gap opening of  $\text{AlH}_3$ . *Physica B: Condensed Matter*, Vol. 411, p. 154, February 2013.
- 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, March 2015.
- Taro Fukazawa, Akihisa Kiyota, and Chuzo Ninagawa. Aggregated transfer function for smart grid FastADR feedback control of wide area distributed building facilities. *IEEE Transactions on Electrical and Electronic Engineering*, Vol. 10, No. 4, p. 487, July 2015.
- Taro Fukazawa, Tomohisa Yamada, and Chuzo Ninagawa. Theoretical performance analysis on trasmission reserve table buffer with triage ranking for resource-limited control networks. *IEEE Transactions on Electrical and Electronic Engineering*, Vol. 11, No. 1, p. 91, January 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. *IEEE Transactions on Electrical and Electronic Engineering*, Vol. 11, No. 1, p. 124, January 2016.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles study of intersite magnetic couplings in  $\text{NdFe}_{12}$  and  $\text{NdFe}_{12}\text{X}$  ( $\text{X} = \text{B}, \text{C}, \text{N}, \text{O}, \text{F}$ ). *Journal of Applied Physics*, Vol. 122, No. 5, p. 053901, August 2017.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles Study of Intersite Magnetic Couplings and Curie Temperature in  $\text{RFe}_{12-x}\text{Cr}_x$  ( $\text{R} = \text{Y}, \text{Nd}, \text{Sm}$ ). *Journal of Physical Society of Japan*, Vol. 87, No. 4, March 2018.
- Yosuke Harashima, Taro Fukazawa, Hiori Kino, and Takashi Miyake. Effect of  $R$ -site substitution and the pressure on stability of  $\text{RFe}_{12}$ : A first-principles study. *Journal of Applied Physics*, Vol. 124, No. 16, p. 163902, October 2018.
- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. First-principles study of spin-wave dispersion in  $\text{Sm}(\text{Fe}_{1-x}\text{Co}_x)_{12}$ . *Journal of Magnetism and Magnetic Materials*, Vol. 469,

pp. 296 – 301, January 2019.

- Taro Fukazawa, Hisazumi Akai, Yosuke Harashima, and Takashi Miyake. Curie temperature of  $\text{Sm}_2\text{Fe}_{17}$  and  $\text{Nd}_2\text{Fe}_{14}\text{B}$ : A first-principles study. *IEEE Transactions on Magnetics*, in press.

## 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 *INSND 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 linearized (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  $\text{AlH}_3$  under high pressure. In *8th Handai Nanoscience and Nanotechnology International Symposium*, Ichō-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  $\text{NdFe}_{12-\delta}\text{M}_\delta$  ( $\text{M} = \text{K-Br}$ ). 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  $\text{Y}_{n-m}\text{Fe}_{5n+2m}$  [(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 spin-wave dispersion in  $\text{Sm}(\text{FeCo})_{12}$ . 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  $\text{ZFe}_{12}$  (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.
- Taro Fukazawa. A machine-learning scheme for searching new rare-earth magnet compounds. In *Sixth Japan-U.S. Bilateral meeting on rare metals*, Washington Marriot Wardman Park, Washington, DC, United States, January 2019. Invited talk.

## 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.  $\text{Y}_{1-x}\text{Lu}_x\text{Mn}_2$  ( $x=0\sim0.05$ ) 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  $\text{YMn}_2$  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.  $\text{YMn}_2$  および  $\text{Y}_{1-x}\text{Lu}_x\text{Mn}_2$  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.  $\text{AlH}_3$  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  $\text{Nd}(\text{Fe}_{12-x}\text{M}_x)\text{X}$  ( $\text{M}=\text{Ti, Co}$ ;  $\text{X}=\text{B, C, N, O, F}$ ) 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  $\text{NdFe}_{12}$  および  $\text{NdFe}_{12}\text{X}$  ( $\text{X} = \text{B}, \text{C}, \text{N}, \text{O}, \text{F}$ ) 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  $\text{NdFe}_{12}$  and  $\text{NdFe}_{12}\text{X}$  ( $\text{X} = \text{B}, \text{C}, \text{N}, \text{O}, \text{F}$ ). 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  $\text{Nd}(\text{Fe}_{12-\delta}\text{M}_{\delta})(\text{M}=\text{K}-\text{Br})$  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  $\text{NdFe}_{12-x}\text{M}_x$  ( $\text{M} = \text{K}-\text{Br}$ ) 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.  $\text{RFe}_{12}$  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  $\text{NdFe}_{12-x}\text{M}_x$  ( $\text{M}=\text{K}-\text{Br}$ ). 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  $\text{RFe}_{12-x}\text{Cr}_x$  ( $\text{R}=\text{Y}, \text{Nd}, \text{Sm}$ ) 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.  $\text{YFe}_{12}\text{N}$  および  $\text{Y}_2\text{Fe}_{17}\text{N}_3$  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  $\text{NdFe}_{12-x}\text{M}_x$  ( $\text{M}=\text{K}-\text{Br}$ ). 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  $\text{RFe}_{12-x}\text{Cr}_x$  ( $\text{R}=\text{Y}, \text{Nd}, \text{Sm}$ ) 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. 希土類-鉄化合物の熱力学的安定性における希土類元素置換と圧力の効果の第一原理的研究. 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.

- Taro Fukazawa. Search for magnet compounds using first-principles calculation and bayesian optimization. MagHEM-ESICMM 磁性材料合同シンポジウム, SYD HALL, Tokyo, Japan, December 2018. Poster presentation.
- 原嶋庸介, 深澤太郎, 木野日織, 三宅隆. ThMn<sub>12</sub> 型希土類-鉄化合物の熱力学的安定性に対する希土類元素置換と圧力の効果. ポスト「京」重点課題 (7)「次世代の産業を支える新機能デバイス・高性能材料の創成 (CDMSI)」第 4 回シンポジウム, The University of Tokyo, Kashiwa, Japan, December 2018. Poster presentation.
- 深澤太郎. 第一原理計算とベイズ最適化を用いた磁石化合物の探索手法. 東京理科大マテリアルズインフォマティクス懇談会キックオフミーティング, 森戸記念館, Tokyo, Japan, February 2019. Poster presentation.

## 賞罰

- Student poster award, June 2010. 3rd-ICNDR: International Conference of Core Research and Engineering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization.
- Best RA award, March 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 Judges’ Selection in “Art in magnetism” contest, April 2018. 2018 IEEE International Magnetism Conference (Intermag2018).