

# List of publications

## 2019

- [1] K. Nakano, R. Maezono and S. Sorella, "All-electron quantum Monte Carlo with Jastrow single determinant Ansatz: application to the sodium dimer", Submitted to *Journal of Chemical Theory and Computation* (2019).
- [2] K. Nakano, T. Konishi and Y. Imamura, "Estimation of maximum absorption wavelength of polymethine dyes in visible and near-infrared region based on time-dependent density functional theory", *Chemical Physics* 518, 15-24 (2019), [doi:10.1016/j.chemphys.2018.11.002](https://doi.org/10.1016/j.chemphys.2018.11.002)
- [3] 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, "High-Pressure Synthesis of  $A_2NiO_2Ag_2Se_2$  ( $A=Sr, Ba$ ) with a High-Spin  $Ni^{2+}$  in Square-Planar Coordination", *Angewandte Chemie International Edition* 58, 756 (2019), [doi:10.1002/anie.201810161](https://doi.org/10.1002/anie.201810161)

## 2018

- [4] K. Nakano and T. Sakai, "Assessing the performance of the Tran-Blaha modified Becke-Jonhson exchange potential for optical constants of semiconductors in the UV-Vis light region", *Journal of Applied Physics* 123, 015104 (2018), [doi:10.1063/1.5006170](https://doi.org/10.1063/1.5006170)

## 2017

- [5] K. Nakano, K. Hongo, and R. Maezono, "Investigation into structural phase transitions in layered titanium-oxypnictides by a computational phonon analysis", *Inorganic chemistry* 56, 13732-13740 (2017), [doi:10.1021/acs.inorgchem.7b01709](https://doi.org/10.1021/acs.inorgchem.7b01709)
- [6] D. Kato, K. Hongo, R. Maezono, M. Higashi, H. Kunioku, M. Yabuuchi, H. Suzuki, H. Okajima, C. Zhong, K. Nakano, R. Abe, and H. Kageyama, "Valence band engineering of layered bismuth oxyhalides toward stable visible-light water splitting: Madelung site potential analysis", *Journal of the American Chemical Society*, 139, 18725 (2017), [doi:10.1021/jacs.7b11497](https://doi.org/10.1021/jacs.7b11497)
- [7] T. Murakami, T. Yamamoto, F. Takeiri, K. Nakano, and H. Kageyama, "Hypervalent Bismuthides  $La_3M\text{Bi}_5$  ( $M = \text{Ti, Zr, Hf}$ ) and Related Antimonides: Absence of Superconductivity", *Inorganic Chemistry* 56, 5041-5045 (2017), [doi:10.1021/acs.inorgchem.7b00031](https://doi.org/10.1021/acs.inorgchem.7b00031)

## 2016

- [8] K. Nakano, K. Hongo, and R. Maezono, "Phonon dispersions and Fermi surfaces nesting explaining the variety of charge ordering in titanium-oxypnictides superconductors", *Scientific Reports* 6, 29661 (2016), [doi:10.1038/srep29661](https://doi.org/10.1038/srep29661)

## 2015

- [9] G. Bouilly, T. Yajima, T. Terashima, W. Yoshimune, K. Nakano, C. Tassel, Y. Kususe, K. Fujita, K. Tanaka, T. Yamamoto, Y. Kobayashi, and H. Kageyama, "Electrical Properties of Epitaxial Thin Films of Oxyhydrides  $\text{ATiO}_{3-x}\text{H}_x$  ( $A = \text{Ba}$  and  $\text{Sr}$ )", *Chemistry of Materials* 27, 6354-6359 (2015), [doi:10.1021/acs.chemmater.5b02374](https://doi.org/10.1021/acs.chemmater.5b02374)

## 2014

- [10] S. Ganesanpotti, T. Yajima, K. Nakano, Y. Nozaki, T. Yamamoto, C. Tassel, Y. Kobayashi, and H. Kageyama, "Superconductivity in  $\text{LaPd}_2\text{As}_2$  with a collapsed 122 structure", *Journal of Alloys and Compounds* 613, 370-374 (2014), [doi:10.1016/j.jallcom.2014.06.054](https://doi.org/10.1016/j.jallcom.2014.06.054)
- [11] S. Ganesanpotti, T. Yajima, T. Tohyama, Z. Li, K. Nakano, Y. Nozaki, C. Tassel, Y. Kobayashi, and H. Kageyama, "LaPd<sub>2</sub>Sb<sub>2</sub>: A pnictide superconductor with  $\text{CaBe}_2\text{Ge}_2$  type structure", *Journal of Alloys and Compounds* 583, 151-154 (2014), [doi:10.1016/j.jallcom.2013.08.005](https://doi.org/10.1016/j.jallcom.2013.08.005)
- [12] T. Yajima, K. Nakano, Y. Nozaki, and H. Kageyama, "Superconducting properties of  $\text{BaTi}_2\text{Pn}_2\text{O}$  ( $\text{Pn} = \text{Sb}, \text{Bi}$ )", *Physica C: Superconductivity and its Applications* 504, 36-38 (2014), [doi:10.1016/j.physc.2014.02.018](https://doi.org/10.1016/j.physc.2014.02.018)

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- [13] T. Yajima, K. Nakano, F. Takeiri, Y. Nozaki, Y. Kobayashi, and H. Kageyama, "Two Superconducting Phases in the Isovalent Solid Solutions  $\text{BaTi}_2\text{Pn}_2\text{O}$  ( $\text{Pn} = \text{As}, \text{Sb}, \text{and Bi}$ )", *Journal of the Physical Society of Japan* 82, 033705 (2013), [doi:10.7566/JPSJ.82.033705](https://doi.org/10.7566/JPSJ.82.033705).
- [14] K. Nakano, T. Yajima, F. Takeiri, M. A. Green, J. Hester, Y. Kobayashi, and H. Kageyama, " $T_c$  Enhancement by Aliovalent Anionic Substitution in Superconducting  $\text{BaTi}_2(\text{Sb}_{1-x}\text{Sn}_x)_2\text{O}$ ", *Journal of the Physical Society of Japan* 82, 074707 (2013), [doi:10.7566/JPSJ.82.074707](https://doi.org/10.7566/JPSJ.82.074707).
- [15] Y. Nozaki, K. Nakano, T. Yajima, H. Kageyama, B. Frandsen, L. Liu, S. Cheung, T. Goko, Y. J. Uemura, T. S. J. Munsie, T. Medina, G. M. Luke, J. Munevar, D. Nishio-Hamane, and C. M. Brown, "Muon spin relaxation and electron/neutron diffraction studies of  $\text{BaTi}_2(\text{As}_{1-x}\text{Sb}_x)_2\text{O}$ : Absence of static magnetism and superlattice reflections", *Physical Review B* 88, 214506 (2013), [doi:10.1103/PhysRevB.88.214506](https://doi.org/10.1103/PhysRevB.88.214506).
- [16] S. Kitagawa, K. Ishida, K. Nakano, T. Yajima, and H. Kageyama "s-wave superconductivity in superconducting  $\text{BaTi}_2\text{Sb}_2\text{O}$  revealed by  $^{121/123}\text{Sb}$ -NMR/nuclear quadrupole resonance measurements", *Physical Review B* 87, 060510(R) (2013), [doi:10.1103/PhysRevB.87.060510](https://doi.org/10.1103/PhysRevB.87.060510)
- [17] G. Hasegawa, T. Sato, K. Kanamori, K. Nakano, T. Yajima, Y. Kobayashi, H. Kageyama, T. Abe, and K. Nakanishi, "Hierarchically porous monoliths based on N-doped reduced titanium oxides and their electric and electrochemical properties" *Chemistry of Materials* 25, 3504-3512 (2013), [doi:10.1021/cm401933a](https://doi.org/10.1021/cm401933a)

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- [19] T. Yajima, K. Nakano, F. Takeiri, T. Ono, Y. Hosokoshi, Y. Matsushita, J. Hester, Y. Kobayashi, and H. Kageyama, "Superconductivity in  $\text{BaTi}_2\text{Sb}_2\text{O}$  with a  $d^1$  square lattice.", *Journal of the Physical Society of Japan* 81, 103706 (2012), [doi:10.1143/JPSJ.81.103706](https://doi.org/10.1143/JPSJ.81.103706).