# Shoji Ishibashi

List of Publications by Year
in descending order

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|---|---|---|---|
| 220 papers | 4,417 citations | 101384 36 h-index | 143772 57 g-index |
| 225 all docs | 225 docs citations | 225 times ranked | 4543 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Effect of solid-solution strengthening on deformation mechanisms and strain hardening in medium-entropy V1-Cr CoNi alloys. Journal of Materials Science and Technology, 2022, 108, 270-280. | 5.6 | 30 |
| 2 | Ferroelectric charge-transfer complexes. , 2022, , 7-46. | | 1 |
| 3 | Hydrogen-bonded organic molecular ferroelectrics/antiferroelectrics. , 2022, , 47-84. | | 3 |
| 4 | Effect of Ultraâ€Highâ€Pressure Annealing on Defect Reactions in Ionâ€Implanted GaN Studied by Positron Annihilation. Physica Status Solidi (B): Basic Research, 2022, 259, . | 0.7 | 7 |
| 5 | A fully automated approach to calculate the melting temperature of elemental crystals. Computational Materials Science, 2021, 187, 110065. | 1.4 | 18 |
| 6 | Reduced nonradiative recombination rates in c-plane Al0.83In0.17N films grown on a nearly lattice-matched GaN substrate by metalorganic vapor phase epitaxy. Applied Physics Letters, 2021, 119, . | 1.5 | 5 |
| 7 | Vacancy-type defects in bulk GaN grown by oxide vapor phase epitaxy probed using positron annihilation. Journal of Crystal Growth, 2021, 570, 126219. | 0.7 | 6 |
| 8 | Single-Component Molecular Conductors â€" Multi-Orbital Correlated Ï€-d Electron Systems. Bulletin of the Chemical Society of Japan, 2021, 94, 2540-2562. | 2.0 | 8 |
| 9 | Hydrogen-bonded single-component organic ferroelectrics revisited by van der Waals density-functional theory calculations. Physical Review Materials, 2021, 5, . | 0.9 | 4 |
| 10 | Large polarization and record-high performance of energy storage induced by a phase change in organic molecular crystals. Chemical Science, 2021, 12, 14198-14206. | 3.7 | 8 |
| 11 | Dopant activation process in Mg-implanted GaN studied by monoenergetic positron beam. Scientific Reports, 2021, 11, 20660. | 1.6 | 12 |
| 12 | Improved minority carrier lifetime in p-type GaN segments prepared by vacancy-guided redistribution of Mg. Applied Physics Letters, 2021, 119, . | 1.5 | 13 |
| 13 | Resonant tunneling driven metal-insulator transition in double quantum-well structures of strongly correlated oxide. Nature Communications, 2021, 12, 7070. | 5.8 | 6 |
| 14 | Vacancy complexes acting as midgap recombination centers in (Al,Ga)N semiconductors. , 2021, , . | | 0 |
| 15 | Effects of ultra-high-pressure annealing on characteristics of vacancies in Mg-implanted GaN studied using a monoenergetic positron beam. Scientific Reports, 2020, 10, 17349. | 1.6 | 22 |
| 16 | Annealing behaviors of vacancy-type defects in AlN deposited by radio-frequency sputtering and metalorganic vapor phase epitaxy studied using monoenergetic positron beams. Journal of Applied Physics, 2020, 128, . | 1.1 | 24 |
| 17 | Hole capture-coefficient of intrinsic nonradiative recombination centers that commonly exist in bulk, epitaxial, and proton-irradiated ZnO. Journal of Applied Physics, 2020, 127, 215704. | 1.1 | 6 |
| 18 | Hydrogen-Bonded Small-Molecular Crystals Yielding Strong Ferroelectric and Antiferroelectric Polarizations. Journal of the Physical Society of Japan, 2020, 89, 051009. | 0.7 | 51 |

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| 19 | Metaelectric multiphase transitions in a highly polarizable molecular crystal. Chemical Science, 2020, 11, 6183-6192. | 3.7 | 7 |
| 20 | Correlation analysis of strongly fluctuating atomic volumes, charges, and stresses in body-centered cubic refractory high-entropy alloys. Physical Review Materials, 2020, 4, . | 0.9 | 17 |
| 21 | Origin and dynamic properties of major intrinsic nonradiative recombination centers in wide bandgap nitride semiconductors. , 2020, , . | | 2 |
| 22 | Control of vacancy-type defects in Mg implanted GaN studied by positron annihilation spectroscopy. , 2020, , . | | 0 |
| 23 | Annealing Behaviours of Open Spaces in Thin Al2O3 Films Deposited on Semiconductors Studied Using Monoenergetic Positron Beams. Acta Physica Polonica A, 2020, 137, 227-230. | 0.2 | 0 |
| 24 | Calculation of Positron States and Annihilation Parameters in Gamma and Amorphous Al2O3. Acta Physica Polonica A, 2020, 137, 231-234. | 0.2 | 1 |
| 25 | Room temperature photoluminescence lifetime for the near-band-edge emission of epitaxial and ion-implanted GaN on GaN structures. Japanese Journal of Applied Physics, 2019, 58, SC0802. | 0.8 | 25 |
| 26 | Computational study of positron annihilation parameters for cation mono-vacancies and vacancy complexes in nitride semiconductor alloys. Journal of Physics Condensed Matter, 2019, 31, 475401. | 0.7 | 14 |
| 27 | First-principles studies of spin-orbital physics in pyrochlore oxides. Journal of Physics Condensed Matter, 2019, 31, 323001. | 0.7 | 12 |
| 28 | Annealing Behavior of Vacancyâ€Type Defects in Mgâ€•and Hâ€Implanted GaN Studied Using Monoenergetic Positron Beams. Physica Status Solidi (B): Basic Research, 2019, 256, 1900104. | 0.7 | 27 |
| 29 | Vacancy-type defects in GaN self-assembled nanowires probed using monoenergetic positron beam. Journal of Applied Physics, 2019, 125, 175705. | 1.1 | 1 |
| 30 | Single-component molecular conductor [Pt(dmdt)<sub>2</sub>]â€”a three-dimensional ambient-pressure molecular Dirac electron system. Chemical Communications, 2019, 55, 3327-3330. | 2.2 | 31 |
| 31 | Vacancy-type defects in GaN-based power device structure - defect characterization in ion implanted GaN and Al2O3/GaN -. , 2019, , . | | 0 |
| 32 | Effect of illumination on positron states in wide bandgap semiconductors. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 33 | Coexistence of normal and inverse deuterium isotope effects in a phase-transition sequence of organic ferroelectrics. RSC Advances, 2019, 9, 39662-39673. | 1.7 | 13 |
| 34 | Hydrogen-Bonded Architectures and Field-Induced Polarization Switching in Bridged Bis(benzimidazole) Crystals. Crystal Growth and Design, 2019, 19, 328-335. | 1.4 | 12 |
| 35 | Field-Induced Antipolarâ€“Polar Structural Transformation and Giant Electrostriction in Organic Crystal. Journal of the American Chemical Society, 2018, 140, 3842-3845. | 6.6 | 22 |
| 36 | Vacancy-type defects in Al2O3/GaN structure probed by monoenergetic positron beams. Journal of Applied Physics, 2018, 123, . | 1.1 | 21 |

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| 37 | Carrier Trapping by Vacancyâ€Type Defects in Mgâ€Implanted GaN Studied Using Monoenergetic Positron Beams. Physica Status Solidi (B): Basic Research, 2018, 255, 1700521. | 0.7 | 60 |
| 38 | Piezoelectricity of strongly polarized ferroelectrics in prototropic organic crystals. Journal of Materials Chemistry C, 2018, 6, 4714-4719. | 2.7 | 26 |
| 39 | The origins and properties of intrinsic nonradiative recombination centers in wide bandgap GaN and AlGaN. Journal of Applied Physics, 2018, 123, . | 1.1 | 112 |
| 40 | Strong polarization switching with low-energy loss in hydrogen-bonded organic antiferroelectrics. Chemical Science, 2018, 9, 425-432. | 3.7 | 41 |
| 41 | (Invited) Vacancy-Type Defects and Their Carrier Trapping Properties in GaN Studied by Monoenergetic Positron Beams. ECS Transactions, 2018, 86, 149-160. | 0.3 | 0 |
| 42 | Large electron capture-cross-section of the major nonradiative recombination centers in Mg-doped GaN epilayers grown on a GaN substrate. Applied Physics Letters, 2018, 112, . | 1.5 | 55 |
| 43 | Computational findings of metastable ferroelectric phases of squaric acid. Physical Review B, 2018, 97, . | 1.1 | 17 |
| 44 | Polarity-dependence of the defect formation in c-axis oriented ZnO by the irradiation of an 8â€‰MeV proton beam. Journal of Applied Physics, 2018, 123, 161562. | 1.1 | 6 |
| 45 | Proton tautomerism for strong polarization switching. Nature Communications, 2017, 8, 14426. | 5.8 | 83 |
| 46 | Prediction of positron-annihilation parameters for vacancy-type defects in ternary alloy semiconductors by data-scientific approach. Journal of Physics: Conference Series, 2017, 791, 012023. | 0.3 | 1 |
| 47 | Nitrogen vacancies as a common element of the green luminescence and nonradiative recombination centers in Mg-implanted GaN layers formed on a GaN substrate. Applied Physics Express, 2017, 10, 061002. | 1.1 | 70 |
| 48 | Electron capture by vacancy-type defects in carbon-doped GaN studied using monoenergetic positron beams. Thin Solid Films, 2017, 639, 78-83. | 0.8 | 11 |
| 49 | Vacancy-type defects in bulk GaN grown by the Na-flux method probed using positron annihilation. Journal of Crystal Growth, 2017, 475, 261-265. | 0.7 | 15 |
| 50 | Antiferromagnetic Mott insulating state in the single-component molecular material Pd(tmdt) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2017, 96, . | 1.1 | 6 |
| 51 | Two-Component Density Functional Study of Positron-Vacancy Interaction in Metals and Semiconductors. Acta Physica Polonica A, 2017, 132, 1602-1605. | 0.2 | 2 |
| 52 | Vacancy-type defects in Mg-implanted GaN probed by a monoenergetic positron beam. , 2016, , . | | 1 |
| 53 | Computational studies of positron states and annihilation parameters in semiconductors â€“ vacancy-type defects in group-III nitrides â€“. Journal of Physics: Conference Series, 2016, 674, 012020. | 0.3 | 8 |
| 54 | Vacancy-type defects in Mg-doped GaN grown by ammonia-based molecular beam epitaxy probed using a monoenergetic positron beam. Journal of Applied Physics, 2016, 119, 245702. | 1.1 | 9 |

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| 55 | First-principles study on stability and magnetism of NdFe11M and NdFe11MN for Mâ€‰=â€‰Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn. Journal of Applied Physics, 2016, 120, . | 1.1 | 62 |
| 56 | Vacancies and electron trapping centers in acidic ammonothermal GaN probed by a monoenergetic positron beam. Journal of Crystal Growth, 2016, 448, 117-121. | 0.7 | 22 |
| 57 | Nitrogen as the best interstitial dopant among<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>X</mml:mi><mml:mo>=</mml:mo><mml:mi mathvariant="normal">B</mml:mi></mml:mrow></mml:math>, C, N, O, and F for strong permanent magnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>NdFe</mml:mi><mml:mn>11</mml:mn></mml:msub></mml:mrow></mml:math>: First-principles study. Physical Review B, 2015, 92, . | 1.1 | 50 |
| 58 | Mechanism of covalency-induced electric polarization within the framework of maximally localized Wannier orbitals. Physical Review B, 2015, 91, . | 1.1 | 18 |
| 59 | Computational Study of Positronâ€“Monovacancy Interaction in d-Block Metals. Journal of the Physical Society of Japan, 2015, 84, 083703. | 0.7 | 6 |
| 60 | Vacancyâ€type defects and their annealing behaviors in Mgâ€implanted GaN studied by a monoenergetic positron beam. Physica Status Solidi (B): Basic Research, 2015, 252, 2794-2801. | 0.7 | 65 |
| 61 | Analysis of Electronic Polarization of Tetragonal BaTiO<sub>3</sub>. , 2015, , . | | 3 |
| 62 | Weyl Node and Spin Texture in Trigonal Tellurium and Selenium. Physical Review Letters, 2015, 114, 206401. | 2.9 | 195 |
| 63 | First-Principles Study of Structural and Magnetic Properties of R(Fe,Ti)<sub>12</sub> and R(Fe,Ti)<sub>12</sub>N (R = Nd, Sm, Y). , 2015, , . | | 13 |
| 64 | Dirac Point in Trigonal Tellurium and Selenium. , 2015, , . | | 0 |
| 65 | Vacancies in In<sub>x</sub>Ga<sub>1â€“</sub><sub>x</sub>N/GaN multiple quantum wells fabricated onm-plane GaN probed by a monoenergetic positron beam. Applied Physics Express, 2015, 8, 051002. | 1.1 | 3 |
| 66 | Correlated Proton Transfer and Ferroelectricity along Alternating Zwitterionic and Nonzwitterionic Anthranilic Acid Molecules. Chemistry of Materials, 2015, 27, 6193-6197. | 3.2 | 16 |
| 67 | First-Principles Study of Magnetocrystalline Anisotropy and Magnetization in NdFe<sub>12</sub>, NdFe<sub>11</sub>Ti, and NdFe<sub>11</sub>TiN. Journal of the Physical Society of Japan, 2014, 83, 043702. | 0.7 | 74 |
| 68 | Structureâ€“Property Relationship of Supramolecular Ferroelectric [Hâ€66dmbp][Hca] Accompanied by High Polarization, Competing Structural Phases, and Polymorphs. Chemistry - A European Journal, 2014, 20, 17515-17522. | 1.7 | 24 |
| 69 | Molecular electronic states in charge transfer complex studied by x-ray absorption spectroscopy. Journal of Physics: Conference Series, 2014, 502, 012036. | 0.3 | 1 |
| 70 | SeoetÂal.Reply:. Physical Review Letters, 2014, 113, 029702. | 2.9 | 3 |
| 71 | Optically active vacancies in GaN grown on Si substrates probed using a monoenergetic positron beam. Applied Physics Letters, 2014, 104, 082110. | 1.5 | 22 |
| 72 | A Single-Component Molecular Superconductor. Journal of the American Chemical Society, 2014, 136, 7619-7622. | 6.6 | 75 |

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| 73 | Polarization Switching Ability Dependent on Multidomain Topology in a Uniaxial Organic Ferroelectric. Nano Letters, 2014, 14, 239-243. | 4.5 | 53 |
| 74 | Second-Order Perturbation Formula for Magnetocrystalline Anisotropy Using Orbital Angular Momentum Matrix. Journal of the Physical Society of Japan, 2014, 83, 044707. | 0.7 | 9 |
| 75 | Native and process induced defects in GaN films grown on Si substrates probed using a monoenergetic positron beam. , 2014, , . | | 0 |
| 76 | Vacancy clusters introduced by CF<sub>4</sub>-based plasma treatment in GaN probed with a monoenergetic positron beam. Applied Physics Express, 2014, 7, 121001. | 1.1 | 5 |
| 77 | Exotic Ferroelectricity in Tetrathiafulvalene-p-Chloranil: Anomalous Effective Charges and a Picture in the Framework of Maximally Localized Wannier Orbitals. Journal of the Physical Society of Japan, 2014, 83, 073702. | 0.7 | 16 |
| 78 | Annealing behaviors of vacancy-type defects near interfaces between metal contacts and GaN probed using a monoenergetic positron beam. Applied Physics Letters, 2014, 105, 052108. | 1.5 | 11 |
| 79 | (Invited) Point Defect Characterization of Group-III Nitrides by Using Monoenergetic Positron Beams. ECS Transactions, 2014, 61, 19-30. | 0.3 | 14 |
| 80 | Ionic versus Electronic Ferroelectricity in Donorâ€“Acceptor Molecular Sequences. Chemistry Letters, 2014, 43, 26-35. | 0.7 | 43 |
| 81 | Defects in nitride-based semiconductors probed by positron annihilation. Journal of Physics: Conference Series, 2014, 505, 012009. | 0.3 | 1 |
| 82 | First-principles calculation of positron states and annihilation parameters for group-III nitrides. Journal of Physics: Conference Series, 2014, 505, 012010. | 0.3 | 33 |
| 83 | Vacancy-type defects in InxGa1â^'xN grown on GaN templates probed using monoenergetic positron beams. Journal of Applied Physics, 2013, 114, . | 1.1 | 15 |
| 84 | Spin-orbital frustration in molybdenum pyrochloresA2Mo2O7(A=rare earth). Physical Review B, 2013, 88, . | 1.1 | 21 |
| 85 | Vacancy-type defects introduced by plastic deformation of GaN studied using monoenergetic positron beams. Journal of Applied Physics, 2013, 114, . | 1.1 | 8 |
| 86 | Origin of surface stress on late transition metal surfaces:Ab initiolocal stress and tight-binding model. Physical Review B, 2013, 87, . | 1.1 | 19 |
| 87 | Point defects introduced by InN alloying into InxGa1â^'xN probed using a monoenergetic positron beam. Journal of Applied Physics, 2013, 113, 123502. | 1.1 | 7 |
| 88 | Positron Annihilation Spectroscopy on Nitride-Based Semiconductors. Japanese Journal of Applied Physics, 2013, 52, 08JJ02. | 0.8 | 26 |
| 89 | Electronic States of Single-Component Molecular Conductors [M(tmdt)<sub>2</sub>]. Journal of the Physical Society of Japan, 2013, 82, 054711. | 0.7 | 16 |
| 90 | Material characterization for advanced Si LSI process technology by means of positron annihilation. Journal of Physics: Conference Series, 2013, 443, 012067. | 0.3 | 1 |

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| 91 | Vacancy-Type Defects Introduced by Gas Cluster Ion-Implantation on Si Studied by Monoenergetic Positron Beams. Japanese Journal of Applied Physics, 2012, 51, 111801. | 0.8 | 2 |
| 92 | Vacancy-type defects in InxGa1â€“xN alloys probed using a monoenergetic positron beam. Journal of Applied Physics, 2012, 112, . | 1.1 | 20 |
| 93 | Tuning the Magnetic Dimensionality by Charge Ordering in the Molecular TMTTF Salts. Physical Review Letters, 2012, 108, 096402. | 2.9 | 36 |
| 94 | Defect characterization in Mg-doped GaN studied using a monoenergetic positron beam. Journal of Applied Physics, 2012, 111, . | 1.1 | 33 |
| 95 | Frustration, Magnetism and Spin-Orbit Coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>5</mml:mn><mml:mi>d</mml:mi></mml:math>Pyrochlore Oxide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cd</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Os</mml:mi><mml:mrow mathvariant="bold">2</mml:mrow><mml:mn>7</mml:mn></mml:msub></mml:math>. Physical Review Lette | 2.9 | 59 |
| 96 | First-Principles Electronic Structure of Superconductor Ca4Al2O6Fe2P2: Comparison with LaFePO and Ca4Al2O6Fe2As2. Journal of the Physical Society of Japan, 2012, 81, 014701. | 0.7 | 5 |
| 97 | Vacancy-type defects introduced by gas cluster ion implantation to Si probed by monoenergetic positron beams. , 2012, , . | | 0 |
| 98 | Native cation vacancies in Si-doped AlGaN studied by monoenergetic positron beams. Journal of Applied Physics, 2012, 111, . | 1.1 | 53 |
| 99 | Electronic Structure of Cu(tmdt)2 Studied with First-Principles Calculations. Crystals, 2012, 2, 1210-1221. | 1.0 | 6 |
| 100 | Firstâ€principles calculations of spontaneous polarization for TTFâ€QBrCl<sub>3</sub>. Physica Status Solidi (B): Basic Research, 2012, 249, 1008-1011. | 0.7 | 3 |
| 101 | Spin-canting in lightly electron-doped CaMnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, . | 1.1 | 12 |
| 102 | Spin frustration, charge ordering, and enhanced antiferromagnetism in TMTTF2SbF6. Physica B: Condensed Matter, 2012, 407, 1783-1786. | 1.3 | 6 |
| 103 | Vacancy-Type Defects Introduced by Gas Cluster Ion-Implantation on Si Studied by Monoenergetic Positron Beams. Japanese Journal of Applied Physics, 2012, 51, 111801. | 0.8 | 3 |
| 104 | Charge-transport in tin-iodide perovskite CH3NH3SnI3: origin of high conductivity. Dalton Transactions, 2011, 40, 5563. | 1.6 | 342 |
| 105 | Impact of Cu/III ratio on the near-surface defects in polycrystalline CuGaSe2 thin films. Applied Physics Letters, 2011, 98, 112105. | 1.5 | 18 |
| 106 | Application of positron annihilation technique to front and backend processes for modern LSI devices. Journal of Physics: Conference Series, 2011, 262, 012061. | 0.3 | 0 |
| 107 | Point defects in GaN and related group-III nitrides studied by means of positron annihilation. Proceedings of SPIE, 2011, , . | 0.8 | 4 |
| 108 | Multi-Orbital Molecular Compound (TTM-TTP)I<sub>3</sub>: Effective Model and Fragment Decomposition. Journal of the Physical Society of Japan, 2011, 80, 013703. | 0.7 | 13 |

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| 109 | Ab initioelectronic structure of solid coronene: Differences from and commonalities to picene. Physical Review B, 2011, 84, . | 1.1 | 37 |
| 110 | First-principles structural optimization and electronic structure of the superconductor picene for various potassium doping levels. Physical Review B, 2011, 84, . | 1.1 | 54 |
| 111 | Slab Thickness Dependence of Rashba Splitting on Au(111) Surface: First-Principles and Model Analyses. Journal of the Physical Society of Japan, 2011, 80, 074713. | 0.7 | 19 |
| 112 | First-Principles Study of Polarizability Distributions for LaAlO3/SrTiO3 Superlattices. Journal of the Physical Society of Japan, 2010, 79, 094701. | 0.7 | 2 |
| 113 | First-Principles Electronic-Structure Study for Organic Ferroelectric Tetrathiafulvaleneâ€“ p-Bromanil. Journal of the Physical Society of Japan, 2010, 79, 043703. | 0.7 | 14 |
| 114 | First-principles study of spontaneous polarization in tetrathiafulvalene-p-chloranil (TTF-CA). Physica B: Condensed Matter, 2010, 405, S338-S340. | 1.3 | 37 |
| 115 | A systematic study of relationship between the Feâ€“As network and electronic structures of SrFe2As2. Physica C: Superconductivity and Its Applications, 2010, 470, S336-S337. | 0.6 | 2 |
| 116 | Defect characterization of crystalline metal oxides and high-k films by means of positron annihilation. , 2010, , . | | 0 |
| 117 | Publisher's Note: Jahn-Teller distortion and magnetic structure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaMnO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> A first-principles theoretical study with full structure optimizations [Phys. Rev. B82, 045124 (2010)]. Physical Review B, 2010, 82, . | 1.1 | 2 |
| 118 | Electronic Structure of Novel Superconductor Ca4Al2O6Fe2As2. Journal of the Physical Society of Japan, 2010, 79, 123713. | 0.7 | 33 |
| 119 | First-Principles Electronic-Structure Study for TTF-TCNQ under Hydrostatic Pressure. Journal of the Physical Society of Japan, 2010, 79, 015001. | 0.7 | 2 |
| 120 | Vacancy-Boron Complexes in Plasma Immersion Ion-Implanted Si Probed by a Monoenergetic Positron Beam. Japanese Journal of Applied Physics, 2010, 49, 051301. | 0.8 | 21 |
| 121 | Jahn-Teller distortion and magnetic structure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaMnO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> A first-principles theoretical study with full structure optimizations. Physical Review B, 2010, 82, . | 1.1 | 53 |
| 122 | First-principles calculations for the magnetic phase diagram in electron-dopedCaMnO3under compressive and tensile strains. Physical Review B, 2010, 81, . | 1.1 | 19 |
| 123 | Effect of V/III flux ratio on luminescence properties and defect formation of Er-doped GaN. Applied Physics Letters, 2010, 96, 051907. | 1.5 | 5 |
| 124 | Ab initiolocal stress and its application to Al (111) surfaces. Physical Review B, 2010, 81, . | 1.1 | 62 |
| 125 | First-principles study of the rectifying properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Pt</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 80, . | 1.1 | 54 |
| 126 | Vacancy-oxygen complexes and their optical properties in AlN epitaxial films studied by positron annihilation. Journal of Applied Physics, 2009, 105, . | 1.1 | 63 |

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| 127 | Vacancy-type defects in Mg-doped InN probed by means of positron annihilation. Journal of Applied Physics, 2009, 105, . | 1.1 | 24 |
| 128 | First-principles electronic-band calculations on organic conductors. Science and Technology of Advanced Materials, 2009, 10, 024311. | 2.8 | 12 |
| 129 | First-Principles Electronic Structure of Solid Picene. Journal of the Physical Society of Japan, 2009, 78, 113704. | 0.7 | 73 |
| 130 | Structures and Physical Properties of Highly Conducting Singleâ€Component Molecular Conductors Containing Se Atoms. European Journal of Inorganic Chemistry, 2009, 2009, 1585-1591. | 1.0 | 8 |
| 131 | Point defects in group-III nitride semiconductors studied by positron annihilation. Journal of Crystal Growth, 2009, 311, 3075-3079. | 0.7 | 51 |
| 132 | First-Principles Study of the Stability and Interfacial Bonding of Tilt and Twist Grain Boundaries in Al and Cu. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2009, 73, 559-565. | 0.2 | 0 |
| 133 | First-Principles Study of the Stability and Interfacial Bonding of Tilt and Twist Grain Boundaries in Al and Cu. Materials Transactions, 2009, 50, 11-18. | 0.4 | 17 |
| 134 | First-principles analysis of optical absorption edge in pure and fluorine-doped SiO2 glass. Computational Materials Science, 2008, 44, 61-66. | 1.4 | 3 |
| 135 | Electronic Structures of Single Component Molecular Metals Based on Ab initio Calculation. Journal of the Physical Society of Japan, 2008, 77, 024702. | 0.7 | 41 |
| 136 | A Possible Ground State and Its Electronic Structure of a Mother Material (LaOFeAs) of New Superconductors. Journal of the Physical Society of Japan, 2008, 77, 053709. | 0.7 | 152 |
| 137 | First-principles analysis of the optical properties of structural disorder in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2008, 77, . | 1.1 | 35 |
| 138 | Vacancy-type defects in Er-doped GaN studied by a monoenergetic positron beam. Journal of Applied Physics, 2008, 103, 104505. | 1.1 | 24 |
| 139 | Analysis of Screening Mechanisms for Polar Discontinuity for LaAlO3/SrTiO3 Thin Films Based on Ab initio Calculations. Journal of the Physical Society of Japan, 2008, 77, 104706. | 0.7 | 37 |
| 140 | Single-Component Molecular Metals as Multiband Ï€â€“d Systems. Journal of the Physical Society of Japan, 2008, 77, 023714. | 0.7 | 36 |
| 141 | A Possible Ground State and Its Electronic Structure of LaFeAsO. Journal of the Physical Society of Japan, 2008, 77, 91-95. | 0.7 | 10 |
| 142 | Static dielectric response and Born effective charge of BN nanotubes fromab initiofinite electric field calculations. Physical Review B, 2007, 75, . | 1.1 | 45 |
| 143 | Annealing properties of vacancy-type defects in ion-implanted GaN studied by monoenergetic positron beams. Journal of Applied Physics, 2007, 102, 084505. | 1.1 | 38 |
| 144 | Vacancy-fluorine complexes and their impact on the properties of metal-oxide transistors with high-k gate dielectrics studied using monoenergetic positron beams. Journal of Applied Physics, 2007, 102, 054511. | 1.1 | 5 |

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