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Publication Metrics

For manuscripts published from date range April 1990 - April 2024

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278

Total Publications

277

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20

Sum of Times Cited by Patents

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Sum of Times Cited by Patents

Publications

For manuscripts published from date range April 1990 - April 2024 (278)

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Metastable atomic-ordered configurations for $\text{Al}_{1/2}\text{Ga}_{1/2}\text{N}$ predicted by Monte-Carlo method based on first-principles calculations

0

Authors (8): Gueriba, Jessiel Siaron; Mizuseki, Hiroshi ... Amano, Hiroshi

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<p>Formation energy crossings in Ga₂O₃-Al₂O₃ quasibinary system: ordered structures and phase transitions in (Al (x) Ga_{1-x})₂O₃</p> <p>Authors (10): Gueriba, Jessiel Siaron; Mizuseki, Hiroshi ... Yoshikawa, Akira</p> <p>Published: Jun 2023 in Japanese Journal of Applied Physics</p> <p>DOI: 10.35848/1347-4065/ACD42C</p>	1
<p>Order-disorder competition in equiatomic 3d-transition-metal quaternary alloys: phase stability and electronic structure</p> <p>Authors (3): Hiroshi Mizuseki; Ryoji Sahara; Kenta Hongo</p> <p>Published: Jan 2023 in Science and Technology of Advanced Materials: Methods</p> <p>DOI: 10.1080/27660400.2022.2153632</p>	<div style="border: 1px solid black; padding: 5px; background-color: #f0f0f0; width: fit-content;"> Not indexed in the Web of Science </div>
<p>High-Throughput Computational Screening of Two-Dimensional Semiconductors</p> <p>Authors (8): Wang, Vei; Tang, Gang ... Geng, Wen Tong</p> <p>Published: Dec 2022 in Journal of Physical Chemistry Letters</p> <p>DOI: 10.1021/ACS.JPCLETT.2C02972</p>	47
<p>Atomistic origin of compositional pulling effect in wurtzite (B, Al, In)_xGa_{1-x}N: A first-principles study</p> <p>Authors (6): Mizuseki, Hiroshi; Gueriba, Jessiel Siaron ... Ohkawa, Kazuhiro</p> <p>Published: Jul 2021 in Journal of Applied Physics</p> <p>DOI: 10.1063/5.0050102</p>	7
<p>Body centered cubic carbon BC14: An all-sp³ bonded full-fledged pentadiamond</p> <p>Authors (3): Wang, Jian-Tao; Chen, Changfeng; Mizuseki, Hiroshi</p> <p>Published: Nov 2020 in Physical Review B</p> <p>DOI: 10.1103/PHYSREVB.102.184106</p>	22
<p>Cmme-SnS: a two-dimensional tin sulfide nanosheet</p> <p>Authors (2): Ram, Babu; Mizuseki, Hiroshi</p> <p>Published: Oct 2020 in Journal of Materials Chemistry A</p> <p>DOI: 10.1039/D0TA05598K</p>	4
<p>C-568: A new two-dimensional sp⁽²⁾-sp⁽³⁾ hybridized allotrope of carbon</p> <p>Authors (2): Ram, Babu; Mizuseki, Hiroshi</p> <p>Published: Mar 2020 in Carbon</p> <p>DOI: 10.1016/J.CARBON.2019.11.062</p>	55
<p>Reactive molecular dynamics simulation of the amorphous carbon growth: Effect of the carbon triple bonds</p> <p>Authors (4): Li, Xiaowei; Mizuseki, Hiroshi ... Lee, Kwang-Ryeol</p> <p>Published: Nov 2019 in Computational Materials Science</p> <p>DOI: 10.1016/J.COMMATSCI.2019.109143</p>	5

A superhard orthorhombic carbon with all six-membered-ring in sp(3) bonding networks Authors (5): Bu, Kun; Wang, Jian-Tao ... Kawazoe, Yoshiyuki Published: Aug 2019 in Physics Letters A DOI: 10.1016/J.PHYSLETA.2019.05.051	18
Accelerated Data-Driven Accurate Positioning of the Band Edges of MXenes Authors (6): Mishra, Avani; Satsangi, Swanti ... Singh, Abhishek K. Published: Feb 2019 in Journal of Physical Chemistry Letters DOI: 10.1021/ACS.JPCLETT.9B00009	41
Strong chromate-adsorbent based on pyrrolic nitrogen structure: An experimental and theoretical study on the adsorption mechanism Authors (8): Ko, Young-Jin; Choi, Keunsu ... Lee, Wook-Seong Published: Nov 2018 in Water Research DOI: 10.1016/J.WATRES.2018.08.033	37
Computational discovery of a new rhombohedral diamond phase Authors (4): Li, Zhen-Zhen; Wang, Jian-Tao ... Chen, Changfeng Published: Sep 2018 in Physical Review B DOI: 10.1103/PHYSREVB.98.094107	31
Orthorhombic carbon oC24: A novel topological nodal line semimetal Authors (7): Li, Zhen-Zhen; Chen, Jia ... Wang, Jian-Tao Published: Jul 2018 in Carbon DOI: 10.1016/J.CARBON.2018.03.003	46
Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene Authors (7): Rajan, Arunkumar Chitteth; Mishra, Avani ... Singh, Abhishek K. Published: Jun 2018 in Chemistry of Materials DOI: 10.1021/ACS.CHEMMATER.8B00686	222
New carbon allotropes in sp + sp ³ bonding networks consisting of C8 cubes Authors (4): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Yoshiyuki Published: Mar 2018 in Physical Chemistry Chemical Physics DOI: 10.1039/C7CP08380G	32
Onion-like carbon as dopant/modification-free electrocatalyst for VO/VO ₂ redox reaction: Performance-control mechanism Authors (8): Ko, Young-Jin; Choi, Keunsu ... Lee, Wook-Seong Published: 2018 in Carbon DOI: 10.1016/J.CARBON.2017.10.073	8
Tetrahexcarbon: A two-dimensional allotrope of carbon Published: 2018 in Carbon DOI: 10.1016/J.CARBON.2018.05.034	87

Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study Authors (7): Mishra, Avnish; Srivastava, Pooja ... Singh, Abhishek K. Published: Aug 2017 in The Journal of Physical Chemistry C DOI: 10.1021/ACS.JPCC.7B06162	40
Chromate adsorption mechanism on nanodiamond-derived onion-like carbon Authors (9): Ko, Young-Jin; Choi, Keunsu ... Lee, Wook-Seong Published: Dec 2016 in Journal of Hazardous Materials DOI: 10.1016/J.JHAZMAT.2016.08.041	22
Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti ₃ C ₂ MXene Authors (5): Srivastava, Pooja; Mishra, Avnish ... Singh, Abhishek K. Published: Sep 2016 in ACS Applied Materials & Interfaces DOI: 10.1021/ACSAMI.6B08413	192
Isolation of pristine MXene from Nb ₄ AlC ₃ MAX phase: a first-principles study Authors (5): Mishra, Avnish; Srivastava, Pooja ... Singh, Abhishek K. Published: Apr 2016 in Physical Chemistry Chemical Physics DOI: 10.1039/C5CP07609A	30
Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp plus sp ² Hybrid Networks Authors (5): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Yoshiyuki Published: Apr 2016 in Scientific Reports DOI: 10.1038/SREP24665	34
Effect of nitrogen doping on titanium carbonitride-derived adsorbents used for arsenic removal Authors (11): Han, Jisun; Lee, Soonjae ... Kang, Shinho Published: Jan 2016 in Journal of Hazardous Materials DOI: 10.1016/J.JHAZMAT.2015.10.001	21
Computational Study on the Interactions of Mustard Gas with Cucurbituril Macrocycles Authors (4): Venkataramanan, Natarajan Sathiyamoorthy; Suvitha, Ambigapathy ... Kawazoe, Yoshiyuki Published: Nov 2015 in International Journal of Quantum Chemistry DOI: 10.1002/QUA.24964	23
The Schottky barrier modulation at PtSi/Si interface by strain and structural deformation Authors (5): Srivastava, Pooja; Shin, Mincheol ... Kim, Seungchul Published: Aug 2015 in AIP Advances DOI: 10.1063/1.4928323	5

Tuning the Electronic and Magnetic Properties of Phosphorene by Vacancies and Adatoms	114
Authors (6): Srivastava, Pooja; Hembram, K. P. S. S. ... Kim, Seungchul	
Published: Mar 2015 in The Journal of Physical Chemistry C	
DOI: 10.1021/JP5110938	
Sources of n-type conductivity in GaInO ₃	11
Authors (6): Wang, V.; Xiao, W. ... Kawazoe, Y.	
Published: Jan 2015 in Journal of Physics D: Applied Physics	
DOI: 10.1088/0022-3727/48/1/015101	
Theoretical evaluation on solubility of synthesized task specific ionic liquids in water	7
Authors (10): Yuvaraj, Surya V. J.; Subbotin, Oleg S. ... Kawazoe, Yoshiyuki	
Published: Dec 2014 in Journal of Molecular Liquids	
DOI: 10.1016/J.MOLLIQ.2014.10.028	
A comparative study of lattice Boltzmann models for incompressible flow	10
Authors (8): Zhang, Liangqi; Zeng, Zhong ... Kawazoe, Yoshiyuki	
Published: Nov 2014 in Computers & Mathematics with Applications	
DOI: 10.1016/J.CAMWA.2014.09.010	
An ideal polymeric C ₆₀ coating on a Si electrode for durable Li-ion batteries	20
Published: Oct 2014 in Carbon	
DOI: 10.1016/J.CARBON.2014.06.049	
Theoretical study of hydrogen storage in binary hydrogen-methane clathrate hydrates	24
Authors (6): Belosludov, R. V.; Zhdanov, R. K. ... Belosludov, V. R.	
Published: Sep 2014 in Journal of Renewable and Sustainable Energy	
DOI: 10.1063/1.4899075	
Hydrogen storage in TiO ₂ functionalized (10,10) single walled carbon nanotube (SWCNT) - First principles study	27
Authors (7): Lavanya, R.; Surya, V. J. ... Kawazoe, Y.	
Published: Mar 2014 in International Journal of Hydrogen Energy	
DOI: 10.1016/J.IJHYDENE.2014.01.048	
Engineering of Band Gap in Metal Organic Frameworks by Functionalizing Organic Linker: A Systematic Density Functional Theory Investigation	86
Authors (6): Pham, Hung Q.; Toan Mai ... Duc Nguyen-Manh	
Published: Mar 2014 in The Journal of Physical Chemistry C	
DOI: 10.1021/JP405997R	
Stability and Composition of Helium Hydrates Based on Ices I-h and II at Low Temperatures	26
Authors (7): Belosludov, Rodion V.; Bozhko, Yulia Y. ... Fomin, Vasily M.	
Published: Feb 2014 in The Journal of Physical Chemistry C	
DOI: 10.1021/JP411241S	

<p>Roles of oxygen vacancy on ferromagnetism in Ni doped In₂O₃: A hybrid functional study</p> <p>Authors (6): Wang, V.; You, C. -Y. ... Kawazoe, Y.</p> <p>Published: Dec 2013 in Journal of Magnetism and Magnetic Materials</p> <p>DOI: 10.1016/J.JMMM.2013.08.001</p>	4
<p>Numerical simulation of crucible rotation in high-temperature solution growth method using a Fourier-Legendre spectral element method</p> <p>Authors (7): Mei, Huan; Zeng, Zhong ... Kawazoe, Yoshiyuki</p> <p>Published: Sep 2013 in International Journal of Heat and Mass Transfer</p> <p>DOI: 10.1016/J.IJHEATMASSTRANSFER.2013.05.018</p>	11
<p>Kinetic Origin of Divergent Decompression Pathways in Silicon and Germanium</p> <p>Authors (4): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Yoshiyuki</p> <p>Published: Apr 2013 in Physical Review Letters</p> <p>DOI: 10.1103/PHYSREVLETT.110.165503</p>	45
<p>A theoretical study of the effects of transition metal dopants on the adsorption and dissociation of hydrogen on nickel clusters</p> <p>Published: Feb 2013 in International Journal of Quantum Chemistry</p> <p>DOI: 10.1002/QUA.24418</p>	20
<p>Controlling 3D Percolation Threshold of Conductor-Insulator Composites by Changing the Granular Size of Insulators</p> <p>Authors (4): Shida, Kazuhito; Sahara, Ryoji ... Kawazoe, Yoshiyuki</p> <p>Published: 2013 in Materials Transactions</p> <p>DOI: 10.2320/MATERTRANS.M2012227</p>	2
<p>Effect of a nickel dimer on the dissociation dynamics of a hydrogen molecule</p> <p>Authors (5): Sahara, Ryoji; Mizuseki, Hiroshi ... Kawazoe, Yoshiyuki</p> <p>Published: 2013 in RSC Advances</p> <p>DOI: 10.1039/C3RA40928G</p>	2
<p>Multi-relaxation-time lattice Boltzmann front tracking method for two-phase flow with surface tension</p> <p>Authors (6): Xie Hai-Qiong; Zhong, Zeng ... Kawazoe, Yoshiyuki</p> <p>Published: Dec 2012 in Chinese Physics B</p> <p>DOI: 10.1088/1674-1056/21/12/124703</p>	9
<p>Modification of graphene as active hydrogen storage medium by strain engineering</p> <p>Authors (4): Surya, V. J.; Iyakutti, K. ... Kawazoe, Y.</p> <p>Published: Dec 2012 in Computational Materials Science</p> <p>DOI: 10.1016/J.COMMATSCI.2012.07.016</p>	21
<p>Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils</p> <p>Published: Nov 2012 in The Journal of Physical Chemistry B</p> <p>DOI: 10.1021/JP3098044</p>	42

<p>Optoelectronic and magnetic properties of Mn-doped indium tin oxide: A first-principles study Published: Oct 2012 in Journal of Applied Physics DOI: 10.1063/1.4757036</p>	9
<p>Transport in quantum spin Hall phase of graphene nanoribbons Published: Sep 2012 in Journal of Applied Physics DOI: 10.1063/1.4754427</p>	1
<p>Three-dimensional unsteady thermocapillary flow under rotating magnetic field Authors (6): Yao, Liping; Zeng, Zhong ... Kawazoe, Yoshiyuki Published: Aug 2012 in Crystal Research and Technology DOI: 10.1002/CRAT.201200029</p>	5
<p>Theoretical investigation of ozone hydrate formation conditions Authors (6): Subbotin, O. S.; Adamova, T. P. ... Belosludov, V. R. Published: Jul 2012 in Journal of Structural Chemistry DOI: 10.1134/S0022476612040026</p>	6
<p>First-principles analysis of structural and opto-electronic properties of indium tin oxide Published: May 2012 in Journal of Applied Physics DOI: 10.1063/1.4719980</p>	16
<p>Insight into the vertical detachment energy oscillation of Na_nC₆₀ – clusters Published: May 2012 in The Journal of Chemical Physics DOI: 10.1063/1.4712219</p>	5
<p>First-principles study of intrinsic defect properties in hexagonal BN bilayer and monolayer Authors (4): Wang, Vei; Ma, Ning ... Kawazoe, Yoshiyuki Published: May 2012 in Solid State Communications DOI: 10.1016/J.SSC.2012.01.034</p>	34
<p>Tuning Electronic Structure of Graphene: A First-Principles Study Authors (4): Surya, V. J.; Iyakutti, K. ... Kawazoe, Y. Published: May 2012 in IEEE Transactions on Nanotechnology DOI: 10.1109/TNANO.2011.2182358</p>	34
<p>Calcium-decorated graphene for hydrogen storage: A van der Waals density functional study Published: Apr 2012 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2011.12.006</p>	27
<p>GW calculations on La₃Ta_{0.5}Ga_{5.5}O₁₄ with oxygen vacancies at non-equivalent sites Published: Mar 2012 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2011.10.036</p>	1

Tantalum Vacancy Effects on Electrical Conductivity of La ₃ Ta _{0.5} Ga _{5.5} O ₁₄ and Ba-based P321 Crystals Authors (4): Chung, Chan-Yeup; Yaokawa, Ritsuko ... Kawazoe, Yoshiyuki Published: Mar 2012 in Key Engineering Materials DOI: 10.4028/WWW.SCIENTIFIC.NET/KEM.508.325	1
First principles calculations of oxygen vacancy in langatate crystal Published: Jan 2012 in Solid State Ionics DOI: 10.1016/J.SSI.2011.10.027	2
Controlling the Percolation Threshold of Conductor-Insulator Composites in a 2D Triangular Lattice by Introducing Binary Size Distributions of Conductor Particles Published: 2012 in Materials Transactions DOI: 10.2320/MATERTRANS.M2012029	2
Theoretical modelling of the phase diagrams of clathrate hydrates for hydrogen storage applications Authors (7): Belosludov, R. V.; Zhdanov, R. K. ... Belosludov, V. R. Published: 2012 in Molecular Simulation DOI: 10.1080/08927022.2011.654204	16
Investigation of convection control under the non-uniform RMF in a liquid bridge Authors (6): Yao, Liping; Zeng, Zhong ... Kawazoe, Yoshiyuki Published: 2012 in Procedia Engineering DOI: 10.1016/J.PROENG.2012.01.1082	2
Thermal Behavior of Caged Silsesquioxane (POSS) Studied by Molecular Dynamics Simulations Authors (6): Abe, Hiroshi; Note, Ryunosuke ... Tomita, Ikuyoshi Published: 2012 in Journal of Inorganic and Organometallic Polymers and Materials DOI: 10.1007/S10904-011-9637-9	11
Band gap engineering of silicene zigzag nanoribbons with perpendicular electric fields: a theoretical study Authors (4): Liang, Yunye; Wang, Vei ... Kawazoe, Yoshiyuki Published: 2012 in Journal of Physics: Condensed Matter DOI: 10.1088/0953-8984/24/45/455302	52
An atomistic level description of guest molecule effect on the formation of hydrate crystal nuclei by ab initio calculations Authors (8): Belosludov, R. V.; Mizuseki, H. ... Belosludov, V. R. Published: 2012 in Journal of Structural Chemistry DOI: 10.1134/S0022476612040014	4

<p>Effects of Alkali Adatoms on CO and H₂S Adsorptions on the Fe(100) Surface: A Density Functional Theory Study Authors (5): Mahyuddin, M. Haris; Belosludov, Rodion V. ... Kawazoe, Yoshiyuki Published: Nov 2011 in The Journal of Physical Chemistry C DOI: 10.1021/JP2071452</p>	18
<p>A first-principles study on water flow through single-walled carbon nanotubes using artificial neural network method Published: Nov 2011 in Journal of Nanoscience and Nanotechnology DOI: 10.1166/JNN.2011.5006</p>	4
<p>First-principles study of the H₂ splitting processes on pure and transition-metal-doped Al (111) surfaces Published: Oct 2011 in International Journal of Hydrogen Energy DOI: 10.1016/J.IJHYDENE.2011.07.052</p>	14
<p>First principles study on desorption of chemisorbed hydrogen atoms from single-walled carbon nanotubes under external electric field Authors (4): Surya, V. J.; Iyakutti, K. ... Kawazoe, Y. Published: Oct 2011 in International Journal of Hydrogen Energy DOI: 10.1016/J.IJHYDENE.2011.08.015</p>	10
<p>Improved Stability and Catalytic Properties of Au₁₆ Cluster Supported on Graphane Published: Sep 2011 in The Journal of Physical Chemistry C DOI: 10.1021/JP207685X</p>	39
<p>Atomistic configurational effects on piezoelectric properties of La₃Ta_{0.5}Ga_{5.5}O₁₄ and a new piezoelectric crystal design Published: Sep 2011 in Acta Materialia DOI: 10.1016/J.ACTAMAT.2011.07.011</p>	2
<p>Single walled carbon nanotubes functionalized with hydrides as potential hydrogen storage media: A survey of intermolecular interactions Authors (5): Surya, V. J.; Iyakutti, K. ... Kawazoe, Y. Published: Sep 2011 in Physica Status Solidi (B) DOI: 10.1002/PSSB.201046532</p>	10
<p>First principles investigation on carbon nanostructures functionalized with borane: An analysis on their hydrogen storage capacity Authors (5): Surya, V. J.; Iyakutti, K. ... Kawazoe, Y. Published: Jun 2011 in Physica E: Low-dimensional Systems and Nanostructures DOI: 10.1016/J.PHYSE.2011.05.003</p>	9
<p>COMPUTATION OF INTERACTION POTENTIAL OF ADSORBATES ON ZIGZAG SWCNTs - APPLICATION TO FUNCTIONALIZATION AND HYDROGEN STORAGE Authors (7): Lakshmi, I.; Silambarasan, D. ... Kawazoe, Y. Published: Jun 2011 in International Journal of Nanoscience DOI: 10.1142/S0219581X11008125</p>	9

Electronic structures and spectra of symmetric meso-substituted porphyrin: DFT and TDDFT-PCM investigations Published: Apr 2011 in International Journal of Quantum Chemistry DOI: 10.1002/QUA.22519	27
Theoretical Study of Solvent Effect on the Structure, First Electronic Excited State, and Nonlinear Optical Properties of Substituted Stilbazolium Cations Authors (4): Inerbaev, Talgat M.; Gu, Feng Long ... Kawazoe, Yoshiyuki Published: Mar 2011 in International Journal of Quantum Chemistry DOI: 10.1002/QUA.22882	5
Effects of hydration level, temperature, side chain and backbone flexibility of the polymer on the proton transfer in short-side-chain perfluorosulfonic acid membranes at low humidity conditions Published: Mar 2011 in Journal of Membrane Science DOI: 10.1016/J.MEMSCI.2010.12.011	14
Effects of rotating magnetic fields on thermocapillary flow in a floating half- zone Authors (7): Yao, Liping; Zeng, Zhong ... Kawazoe, Yoshiyuki Published: Feb 2011 in Journal of Crystal Growth DOI: 10.1016/J.JCRYSGRO.2010.12.065	13
Conductivity Percolation on a Cubic Lattice with Two Different Sizes of Particles Published: 2011 in Materials Transactions DOI: 10.2320/MATERTRANS.M2010310	1
Electron transport characteristics of organic molecule encapsulated carbon nanotubes Published: 2011 in Nanoscale DOI: 10.1039/C0NR00757A	9
Conductivity Percolation on a Cubic Lattice with Core-Shell Particles Published: 2011 in Materials Transactions DOI: 10.2320/MATERTRANS.M2010412	1
Gate-controlled current and inelastic electron tunneling spectrum of benzene: A self-consistent study Published: 2011 in The Journal of Chemical Physics DOI: 10.1063/1.3571475	9
Hydrogenation-chain-opened conductive channels in zigzag graphene nanoribbons Authors (7): Wu, D. D.; Jiang, F. ... Kawazoe, Y. Published: 2011 in Journal of Applied Physics DOI: 10.1063/1.3614496	5

Impact of type of crystal defects in multicrystalline Si on electrical properties and interaction with impurities Published: 2011 in Journal of Applied Physics DOI: 10.1063/1.3544208	20
Controlling 3D Percolation Threshold of Conductor-Insulator Composites by Changing the Granular Size of Conductors Published: 2011 in Materials Transactions DOI: 10.2320/MATERTRANS.M2011176	3
Thermodynamic stability of C ₃ H ₈ hydrate of cubic structure IV using lattice dynamics Authors (6): Souissi, Maaouia; Belosludov, Rodion V. ... Belosludov, Vladimir R. Published: 2011 in Journal of Inclusion Phenomena and Macrocyclic Chemistry DOI: 10.1007/S10847-010-9845-X	1
On the kinetics of the capillary imbibition of a simple fluid through a designed nanochannel using the molecular dynamics simulation approach Authors (3): Ahadian, Samad; Mizuseki, Hiroshi; Kawazoe, Yoshiyuki Published: Dec 2010 in Journal of Colloid and Interface Science DOI: 10.1016/J.JCIS.2010.09.011	22
First principles calculation of La ₃ Ta _{0.5} Ga _{5.5} O ₁₄ crystal with acceptor-like intrinsic point defects Published: Dec 2010 in Journal of Applied Physics DOI: 10.1063/1.3514008	11
Effects of rotating magnetic fields on thermocapillary flow: Comparison of the infinite and the Phi(1)-Phi(2) models Authors (4): Yao, Liping; Zeng, Zhong ... Kawazoe, Yoshiyuki Published: Dec 2010 in International Journal of Thermal Sciences DOI: 10.1016/J.IJTHERMALSCI.2010.07.017	11
Theoretical investigation on the alkali-metal doped BN fullerene as a material for hydrogen storage Published: Nov 2010 in Chemical Physics DOI: 10.1016/J.CHEMPHYS.2010.08.015	36
Thermodynamic phase behavior of binary clathrate hydrates: Computational prediction Published: Oct 2010 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2010.02.017	10
Theoretical investigation of hydrogen storage ability of a carbon nanohorn Published: Oct 2010 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2009.12.013	12

Quantum chemical study on the alkali atom doped calix[4]arene as hydrogen storage material Authors (4): Venkataramanan, Natarajan Sathiyamoorthy; Sahara, Ryoji ... Kawazoe, Yoshiyuki Published: Oct 2010 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2010.01.028	7
Modular, Homochiral, Porous Coordination Polymers: Rational Design, Enantioselective Guest Exchange Sorption and Ab Initio Calculations of Host-Guest Interactions Authors (13): Dybtsev, Danil N.; Yutkin, Maxim P. ... Belosludov, Vladimir R. Published: Sep 2010 in Chemistry - A European Journal DOI: 10.1002/CHEM.201000522	72
Self-Consistent Study of Conjugated Aromatic Molecular Transistors Authors (7): Wang Jing; Liang Yun-Ye ... Kawazoe, Y. Published: Jun 2010 in Chinese Physics Letters DOI: 10.1088/0256-307X/27/6/067303	3
Titanium-Doped Nickel Clusters TiN _n (n=1-12): Geometry, Electronic, Magnetic, and Hydrogen Adsorption Properties Authors (4): Venkataramanan, Natarajan Sathiyamoorthy; Sahara, Royoji ... Kawazoe, Yoshiyuki Published: Apr 2010 in The Journal of Physical Chemistry A DOI: 10.1021/JP100459C	51
First-Principles Calculations on Σ3 Grain Boundary Transition Metal Impurities in Multicrystalline Silicon Published: Apr 2010 in Japanese Journal of Applied Physics - Special Issues DOI: 10.1143/JJAP.49.04DP02	7
The Origin of the Halogen Effect on the Phthalocyanine Green Pigments Published: Apr 2010 in Chemistry - An Asian Journal DOI: 10.1002/ASIA.200900601	20
Theoretical insights into the formation, structure, and electronic properties of anticancer oxaliplatin drug and cucurbit[n]urils n=5 to 8 Authors (5): Suvitha, Ambigapathy; Venkataramanan, Natarajan Sathiyamoorthy ... Ohuchi, Nobiki Published: Apr 2010 in Journal of Inclusion Phenomena and Macrocyclic Chemistry DOI: 10.1007/S10847-009-9601-2	55
Atomistic nucleation and growth mechanism for single-wall carbon nanotubes on catalytic nanoparticle surfaces Authors (8): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Yoshiyuki Published: Mar 2010 in Nanotechnology DOI: 10.1088/0957-4484/21/11/115602	6

Phase stability of carbon clathrates at high pressure Authors (5): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Y. Published: Mar 2010 in Journal of Applied Physics DOI: 10.1063/1.3359682	35
The role of Li and Ni metals in the adsorbate complex and their effect on the hydrogen storage capacity of single walled carbon nanotubes coated with metal hydrides, LiH and NiH ₂ Authors (5): Surya, V. J.; Iyakutti, K. ... Kawazoe, Y. Published: Mar 2010 in International Journal of Hydrogen Energy DOI: 10.1016/J.IJHYDENE.2010.01.001	34
Correlation between microhardness and electronic charge density of hafnium hydrides Authors (8): Tsuchiya, B.; Sahara, R. ... Kawazoe, Y. Published: Jan 2010 in Journal of Alloys and Compounds DOI: 10.1016/J.JALLCOM.2009.09.151	4
Reducible and non-reducible defect clusters in tin-doped indium oxide Authors (5): Inerbaev, Talgat M.; Sahara, Ryoji ... Nakamura, Takashi Published: Jan 2010 in Solid State Communications DOI: 10.1016/J.SSC.2009.10.016	5
Rigid adamantane tripod linkage for well-defined conductance of a single-molecule junction Published: 2010 in Physical Chemistry Chemical Physics DOI: 10.1039/C001400A	12
Conductivity Percolation on a Square Lattice with Core-Shell Particles Published: 2010 in Materials Transactions DOI: 10.2320/MATERTRANS.M2009329	4
Electron transport characteristics of one-dimensional heterojunctions with multi-nitrogen-doped capped carbon nanotubes Published: 2010 in Nanoscale DOI: 10.1039/C0NR00411A	8
First-principles study of structural stability, magnetism, and hyperfine coupling in hydrogen clusters adsorbed on graphene Authors (5): Ranjbar, Ahmad; Bahramy, Mohammad Saeed ... Kawazoe, Yoshiyuki Published: 2010 in Physical Review B DOI: 10.1103/PHYSREVB.82.165446	45
Prediction and analysis of flow behavior of a polymer melt through nanochannels using artificial neural network and statistical methods Authors (3): Ahadian, Samad; Mizuseki, Hiroshi; Kawazoe, Yoshiyuki Published: 2010 in Microfluidics and Nanofluidics DOI: 10.1007/S10404-009-0549-8	13

Controlling the Percolation Threshold of Conductor-Insulator Composites by Changing the Granular Size of Insulators Published: 2010 in Materials Transactions DOI: 10.2320/MATERTRANS.M2010019	11
A novel computational approach to study proton transfer in perfluorosulfonic acid membranes Authors (4): Ahadian, Samad; Ranjbar, Ahmad ... Kawazoe, Yoshiyuki Published: 2010 in International Journal of Hydrogen Energy DOI: 10.1016/J.IJHYDENE.2010.01.095	11
Accurate description of phase diagram of clathrate hydrates at the molecular level Authors (5): Belosludov, Rodion V.; Subbotin, Oleg S. ... Belosludov, Vladimir R. Published: Dec 2009 in The Journal of Chemical Physics DOI: 10.1063/1.3276282	44
Polarization-induced switching effect in graphene nanoribbon edge-defect junction Authors (8): Yin, G.; Liang, Y. Y. ... Kawazoe, Y. Published: Dec 2009 in The Journal of Chemical Physics DOI: 10.1063/1.3273312	11
Hydrogen storage capacity of C-60(OM)(12) (M=Li and Na) clusters Authors (4): Peng, Qi; Chen, Gang ... Kawazoe, Yoshiyuki Published: Dec 2009 in The Journal of Chemical Physics DOI: 10.1063/1.3268919	40
Conductivity Percolation on a Square Lattice with Two Different Sizes of Particles Authors (5): Shida, Kazuhito; Sahara, Ryoji ... Kawazoe, Yoshiyuki Published: Dec 2009 in Materials Transactions DOI: 10.2320/MATERTRANS.M2009202	7
An efficient tool for modeling and predicting fluid flow in nanochannels Authors (3): Ahadian, Samad; Mizuseki, Hiroshi; Kawazoe, Yoshiyuki Published: Nov 2009 in The Journal of Chemical Physics DOI: 10.1063/1.3253701	9
Chemical engineering of prehydrogenated C and BN-sheets by Li: Application in hydrogen storage Authors (5): Khazaei, Mohammad; Bahramy, Mohammad Saeed ... Kawazoe, Yoshiyuki Published: Nov 2009 in Journal of Applied Physics DOI: 10.1063/1.3247342	38

Geometrical indications of adsorbed hydrogen atoms on graphite producing star and ellipsoidal like features in scanning tunneling microscopy images: Ab initio study Authors (5): Khazaei, Mohammad; Bahramy, Mohammad Saeed ... Kawazoe, Yoshiyuki Published: Nov 2009 in Carbon DOI: 10.1016/J.CARBON.2009.07.051	23
HYDROGEN STORAGE ON NANOFULLERENE CAGES Authors (3): Venkataramanan, Natarajan Sathiyamoorthy; Mizuseki, Hiroshi; Kawazoe, Yoshiyuki Published: Oct 2009 in Nano DOI: 10.1142/S1793292009001733	17
Theoretical study of phase transitions in Kr and Ar clathrate hydrates from structure II to structure I under pressure Authors (8): Subbotin, Oleg S.; Adamova, Tatiana P. ... Belosludov, Vladimir R. Published: Sep 2009 in The Journal of Chemical Physics DOI: 10.1063/1.3212965	37
Designing Nanogadgetry for Nanoelectronic Devices with Nitrogen-Doped Capped Carbon Nanotubes Authors (4): Lee, Sang Uck; Belosludov, Rodion V. ... Kawazoe, Yoshiyuki Published: Aug 2009 in Small DOI: 10.1002/SMLL.200801938	167
TD-DFT Studies on Hematoporphyrin and Its Dimers Authors (7): Suvitha, A.; Belosludov, R. V. ... Ohuchi, N. Published: Aug 2009 in Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals DOI: 10.2320/JJINSTMET.73.555	0
First-principles study of hydrogen storage over Ni and Rh doped BN sheets Authors (5): Venkataramanan, Natarajan Sathiyamoorthy; Khazaei, Mohammad ... Kawazoe, Yoshiyuki Published: May 2009 in Chemical Physics DOI: 10.1016/J.CHEMPHYS.2009.04.001	80
Probing the Structure, Stability and Hydrogen Adsorption of Lithium Functionalized Isoreticular MOF-5 (Fe, Cu, Co, Ni and Zn) by Density Functional Theory Authors (4): Venkataramanan, Natarajan Sathiyamoorthy; Sahara, Ryoji ... Kawazoe, Yoshiyuki Published: Apr 2009 in International Journal of Molecular Sciences DOI: 10.3390/IJMS10041601	24
Highly stable and symmetric boron caged B@Co ₁₂ @B ₈₀ core-shell cluster Authors (6): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Y. Published: Mar 2009 in Applied Physics Letters DOI: 10.1063/1.3111444	9

A theoretical study on the interaction of aromatic amino acids with graphene and single walled carbon nanotube Authors (4): Rajesh, Chinagandham; Majumder, Chiranjib ... Kawazoe, Yoshiyuki Published: Mar 2009 in The Journal of Chemical Physics DOI: 10.1063/1.3079096	219
Understanding of Electroconductivity of Thin Film Using Percolation Model, for Reduction in Indium Consumption Authors (4): Shida, Kazuhito; Sahara, Ryoji ... Kawazoe, Yoshiyuki Published: Mar 2009 in Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals DOI: 10.2320/JINSTMET.73.171	1
THERMODYNAMICS AND HYDROGEN STORAGE ABILITY OF BINARY HYDROGEN Authors (6): Belosludov, V. R.; Subbotin, O. S. ... Kudoh, J. Published: Feb 2009 in International Journal of Nanoscience DOI: 10.1142/S0219581X0900589X	3
Observation of birefringence in BBO crystals in the terahertz regime Authors (11): Saito, Shigeki; Estacio, Elmer ... Kawazoe, Yoshiyuki Published: Jan 2009 in Journal of Crystal Growth DOI: 10.1016/J.JCRYSGRO.2008.09.130	4
Hydrogen Adsorption on Lithium-Functionalized Calixarenes: A Computational Study Published: Nov 2008 in The Journal of Physical Chemistry C DOI: 10.1021/JP808899T	28
Thermocapillary Convection of Liquid Bridge under Axisymmetric Magnetic Fields Authors (4): Chen, Chaobo; Zeng, Zhong ... Kawazoe, Yoshiyuki Published: Nov 2008 in Materials Transactions DOI: 10.2320/MATERTRANS.MB200830	6
Crystal-like low frequency phonons in the low-density amorphous and high-density amorphous ices Published: Sep 2008 in The Journal of Chemical Physics DOI: 10.1063/1.2977975	8
Excess polarizabilities upon the first dipole-allowed excitation of some conjugated oligomers Published: Sep 2008 in Journal of Physical Organic Chemistry DOI: 10.1002/POC.1378	1
Effect of strain on the energetics and kinetics of dissociation of Sb4 on Ge(001) Authors (6): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Y. Published: Aug 2008 in Physical Review B DOI: 10.1103/PHYSREVB.78.073403	4

The Role of Aromaticity and the π -Conjugated Framework in Multiporphyrinic Systems as Single-Molecule Switches Published: Jul 2008 in Small DOI: 10.1002/SMLL.200701220	27
Transport Properties of Nanoscale Materials for Molecular Wire Applications: A Case Study of Ferrocene Dimers Published: Apr 2008 in Journal of the Korean Physical Society DOI: 10.3938/JKPS.52.1197	11
Temperature Dependence of the Bulk Modulus in fcc Metals by Using a Lattice-Gas Model with Renormalized Potentials Published: Apr 2008 in Journal of the Korean Physical Society DOI: 10.3938/JKPS.52.1259	2
Birefringence of β -BaB ₂ O ₄ crystal in the terahertz region for parametric device design Authors (10): Estacio, Elmer; Saito, Shigeki ... Kawazoe, Yoshiyuki Published: Mar 2008 in Applied Physics Letters DOI: 10.1063/1.2890727	21
First-principles study of length dependence of conductance in alkanedithiols Published: Jan 2008 in The Journal of Chemical Physics DOI: 10.1063/1.2827868	28
TD-DFT Studies on Hematoporphyrin and Its Dimers Published: 2008 in Materials Transactions DOI: 10.2320/MATERTRANS.MB200829	6
Structural Dependence of Magnetic Shielding Properties in Al ₄ Li ₄ Clusters Published: 2008 in Materials Transactions DOI: 10.2320/MATERTRANS.MB200823	0
Realization of a computer simulation environment based on ITBL and a large scale GW calculation performed on this platform Authors (9): Kawazoe, Yoshiyuki; Sluiter, Marcel ... Yamaguchi, Hiroshi Published: 2008 in Lecture Notes in Computer Science DOI: 10.1007/978-3-540-77704-5_40	0
Current through single conjugated molecules: Calculations versus measurements Published: 2008 in The Journal of Chemical Physics DOI: 10.1063/1.2951986	8
Control of Electron Transport by Manipulating the Conjugated Framework Published: Oct 2007 in The Journal of Physical Chemistry C DOI: 10.1021/JP074294N	24

Proposed design principle of fluoride-based materials for deep ultraviolet light emitting devices Published: Sep 2007 in Optical Materials DOI: 10.1016/J.OPTMAT.2006.11.031	41
Quantum length dependence of conductance in oligomers: First-principles calculations Published: Jun 2007 in Physical Review B DOI: 10.1103/PHYSREVB.75.245407	35
Interstitial oxygen and dopant atoms arrangement in tin-doped indium oxide Authors (5): Inerbaev, Talgat M.; Sahara, Ryoji ... Nakamura, Takashi Published: Apr 2007 in Materials Transactions DOI: 10.2320/MATERTRANS.48.666	11
Interpreting STM image and tunneling-current-induced rotation of cis-2-butene on a Pd(110) surface Published: Feb 2007 in Chemical Physics Letters DOI: 10.1016/J.CPLETT.2006.12.039	3
Gate-induced switching and negative differential resistance in a single-molecule transistor: Emergence of fixed and shifting states with molecular length Authors (6): Farajian, A. A.; Belosludov, R. V. ... Yakobson, B. I. Published: 2007 in The Journal of Chemical Physics DOI: 10.1063/1.2748047	25
Calculating Transport Properties of Nanometer-Scale Systems: Nanodevice Applications of Carbon Nanotubes and Organic Molecules Authors (5): Farajian, Amir A.; Belosludov, Rodion V. ... Kawazoe, Yoshiyuki Published: 2007 in NanoScience and Technology DOI: 10.1007/978-3-540-37578-4_6	1
Ab initio study of single-molecule rotation switch based on nonequilibrium Green's function theory Authors (7): Liang, Y. Y.; Jiang, F. ... Kawazoe, Y. Published: 2007 in The Journal of Chemical Physics DOI: 10.1063/1.2771156	15
Influence of molecular geometry, exchange-correlation functional, and solvent effects in the modeling of vertical excitation energies in phthalocyanines using time-dependent density functional theory (TDDFT) and polarized continuum model TDDFT methods: Can modern computational chemistry methods explain experimental controversies? Authors (5): Nemykin, Victor N.; Hadt, Ryan G. ... Kawazoe, Yoshiyuki Published: 2007 in The Journal of Physical Chemistry A DOI: 10.1021/JP0759731	152
CO Oxidation Process on Pt-M(111) Alloys (M=Ru, Sn): An ab initio Study Published: 2007 in Materials Transactions DOI: 10.2320/MATERTRANS.N-MRA2007858	1

Special Issue on ACCMS Working Group Meeting on Clusters and Nanomaterials - Preface Published: 2007 in Materials Transactions	0
Excess polarizabilities upon excitation from the ground state to the first dipole-allowed excited state of diphenylpolyenes Published: 2007 in International Journal of Quantum Chemistry DOI: 10.1002/QUA.21361	10
Electronic and transport properties of bismuth nanolines for applications in molecular electronics Authors (5): Belosludov, R. V.; Farajian, A. A. ... Kawazoe, Y. Published: 2007 in Physical Review B DOI: 10.1103/PHYSREVB.75.113411	25
Vacancy induced structural and magnetic transition in MnCo _{1-x} Ge Authors (7): Wang, Jian-Tao; Wang, Ding-Sheng ... Kawazoe, Y. Published: Dec 2006 in Applied Physics Letters DOI: 10.1063/1.2424273	129
First-principles study of phenyl ethylene oligomers as current-switch Published: Dec 2006 in Physics Letters A DOI: 10.1016/J.PHYSLETA.2006.06.070	36
Self-consistent study of single molecular transistor modulated by transverse field Published: Aug 2006 in The Journal of Chemical Physics DOI: 10.1063/1.2337286	17
Two-stage rotation mechanism for group-v precursor dissociation on Si(001) Authors (6): Wang, Jian-Tao; Chen, Changfeng ... Kawazoe, Y. Published: Jul 2006 in Physical Review Letters DOI: 10.1103/PHYSREVLETT.97.046103	11
Dynamic formation process of Bi line structure on S(100) surface Authors (7): Wang, JT; Wang, DS ... Nishigaki, S Published: May 2006 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2005.02.016	0
Electronic and magnetic properties of double-impurities-doped TiO ₂ (rutile): First-principles calculations Published: Apr 2006 in Journal of Applied Physics DOI: 10.1063/1.2165108	10
Excited state properties and quadratic optical nonlinearities in charged organic chromophores: Theoretical analysis Authors (6): Inerbaev, Talgat M.; Saito, Shigeki ... Kawazoe, Yoshiyuki Published: 2006 in The Journal of Chemical Physics DOI: 10.1063/1.2403864	4

First-principles calculations of the far-infrared absorption spectrum of 4'-dimethylamino-N-methyl-4-stilbazolium tosylate Authors (6): Saito, Shigeki; Inerbaev, Talgat M. ... Kawazoe, Yoshiyuki Published: 2006 in Chemical Physics Letters DOI: 10.1016/J.CPLETT.2006.10.089	26
Surface and bulklike phonon modes of Si(100) nanometer thin film Authors (6): Saito, Shigeki; Inerbaev, Talgat M. ... Kawazoe, Yoshiyuki Published: 2006 in Chemical Physics Letters DOI: 10.1016/J.CPLETT.2006.11.047	2
First excited state properties and static hyperpolarizability of ruthenium(II) ammine complexes Authors (5): Inerbaev, Talgat M.; Belosludov, Rodion V. ... Kawazoe, Yoshiyuki Published: 2006 in Journal of Chemical Theory and Computation DOI: 10.1021/CT050193M	26
Electronic and transport properties of ferrocene: Theoretical study Authors (5): Uehara, T; Belosludov, RV ... Kawazoe, Y Published: 2006 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.45.3768	15
Interaction of single-walled carbon nanotubes with alkylamines: An ab initio study Authors (5): Pupysheva, OV; Farajian, AA ... Kawazoe, Y Published: 2006 in Thin Solid Films DOI: 10.1016/J.TSF.2005.07.021	10
Terahertz vibrational modes of crystalline salicylic acid by numerical model using periodic density functional theory Authors (5): Saito, Shigeki; Inerbaev, Talgat M. ... Kawazoe, Yoshiyuki Published: 2006 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.45.4170	20
Cs doping effects on electronic structure of thin nanotubes Authors (4): Khazaei, M; Farajian, AA ... Kawazoe, Y Published: 2006 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2005.03.024	9
Terahertz phonon modes of an intermolecular network of hydrogen bonds in an anhydrous beta-D-glucopyranose crystal Authors (6): Saito, Shigeki; Inerbaev, Talgat M. ... Kawazoe, Yoshiyuki Published: 2006 in Chemical Physics Letters DOI: 10.1016/J.CPLETT.2006.04.012	37
Activation Barriers of CO Oxidation on Pt-M(M=Ru, Sn) Alloys Published: 2006 in Journal of the Japan Institute of Metals DOI: 10.2320/JJINSTMET.70.495	5

Realization of molecular interconnection for molecular electronics: Theoretical aspects Authors (5): Belosludov, RV; Farajian, AA ... Kawazoe, Y Published: 2006 in Computational Materials Science DOI: 10.1016/J.COMMATSCI.2004.11.012	18
Transition between N- and Z-shaped current-voltage characteristics in semiconductor multiple-quantum-well structures Authors (5): Pupysheva, O. V.; Dmitriev, A. V. ... Kawazoe, Y. Published: 2006 in Journal of Applied Physics DOI: 10.1063/1.2234546	10
First principles calculation of terahertz vibrational modes of a disaccharide monohydrate crystal of lactose Authors (6): Saito, Shigeki; Inerbaev, Talgat M. ... Kawazoe, Yoshiyuki Published: 2006 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.45.L1156	21
A general-purpose approach for calculating transport in contact-molecule- contact systems: TARABORD implementation and application to a polythiophene-based nanodevice Authors (4): Farajian, AA; Belosludov, RV ... Kawazoe, Y Published: 2006 in Thin Solid Films DOI: 10.1016/J.TSF.2005.07.122	32
Theoretical study of conductance properties of metallocene Authors (6): Uehara, Tornoki; Igarashi, Nobuaki ... Kawazoe, Yoshiyuki Published: 2006 in Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals DOI: 10.2320/JJINSTMET.70.478	2
Theoretical study on junctions in porphyrin oligomers for nanoscale devices Authors (5): Mizuseki, H; Belosludov, RV ... Kawazoe, Y Published: Dec 2005 in Materials Science and Engineering: C DOI: 10.1016/J.MSEC.2005.07.012	5
Ab initio study of molecule transport characteristics based on nonequilibrium Green's function theory Published: Oct 2005 in Physical Review B DOI: 10.1103/PHYSREVB.72.155408	28
Band-Structure Design of Fluoride Complex Materials for Deep-Ultraviolet Light-Emitting Diodes Published: Oct 2005 in Japanese Journal of Applied Physics - Special Issues DOI: 10.1143/JJAP.44.7285	18
Ab initio study of strain-induced ferroelectricity in SrTiO ₃ Authors (6): Hashimoto, T; Nishimatsu, T ... Ikeda, Y Published: Sep 2005 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.44.7134	10

<p>Dynamic ad-dimer twisting assisted nanowire self-assembly on Si(001) Authors (7): Wang, JT; Wang, EG ... Nishigaki, S Published: Jun 2005 in Physical Review Letters DOI: 10.1103/PHYSREVLETT.94.226103</p>	22
<p>Electronic and transport properties of doped organic molecules for molecular wire applications Authors (5): Belosludov, RV; Farajian, AA ... Kawazoe, Y Published: Apr 2005 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.44.2823</p>	11
<p>Atomic and electronic structures of neutral and cation S_n ($n=2-20$) clusters: A comparative theoretical study with different exchange-correlation functionals -: art. no. 035401 Authors (4): Majumder, C; Kumar, V ... Kawazoe, Y Published: Jan 2005 in Physical Review B DOI: 10.1103/PHYSREVB.71.035401</p>	41
<p>Electron transport through molecular wire: effect of isomery Published: Jan 2005 in Physica E: Low-dimensional Systems and Nanostructures DOI: 10.1016/J.PHYSE.2004.09.006</p>	8
<p>Thermodynamic Properties of Transition Metals Using Face-Centered-Cubic Lattice Model with Renormalized Potentials Published: 2005 in Materials Transactions DOI: 10.2320/MATERTRANS.46.1127</p>	4
<p>An ab initio study of single-walled nanotubes bombarded with 50-150 eV Cs+ ions Authors (4): Khazaei, M; Farajian, AA ... Kawazoe, Y Published: 2005 in Chemical Physics Letters DOI: 10.1016/J.CPLETT.2005.08.118</p>	5
<p>TiO₂ (rutile) doped with double impurities for fabricating spintronic devices —a combinatorial computational approach Published: 2005 in Measurement Science and Technology DOI: 10.1088/0957-0233/16/1/032</p>	6
<p>Design of wide-gap fluoride heterostructures for deep ultraviolet optical devices Authors (14): El Ouenzerfi, R; Ono, S ... Fukuda, T Published: Dec 2004 in Journal of Applied Physics DOI: 10.1063/1.1808474</p>	26
<p>Structure and electronic properties of metal di-(4-thiophenyl)-porphyrin Authors (6): Kikuchi, Y; Belosludov, RV ... Kawazoe, Y Published: Nov 2004 in Molecular Simulation DOI: 10.1080/08927020412331298667</p>	1

<p>Energetics and local spin magnetic moment of single 3,4d impurities encapsulated in an icosahedral Au₁₂ cage -: art. no. 165413 Authors (6): Wang, SY; Yu, JZ ... Kawazoe, Y Published: Oct 2004 in Physical Review B DOI: 10.1103/PHYSREVB.70.165413</p>	78
<p>Ab initio determination of total-energy surfaces for distortions of ferroelectric perovskite oxides Authors (6): Hashimoto, T; Nishimatsu, T ... Ikeda, Y Published: Sep 2004 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.43.6785</p>	12
<p>Current-Voltage Characteristics of Molecular Devices at Low Bias Published: Jul 2004 in Chinese Physics Letters DOI: 10.1088/0256-307X/21/7/017</p>	0
<p>Effect of substituent groups on the electronic properties of a molecular device: an ab initio theoretical study Published: Jul 2004 in Computational and Theoretical Chemistry DOI: 10.1016/J.THEOCHEM.2004.05.013</p>	26
<p>Electron transport through heterocyclic molecule: ab initio molecular orbital theory Published: Jun 2004 in Physics Letters A DOI: 10.1016/J.PHYSLETA.2004.04.043</p>	9
<p>Three-dimensional unsteady convection in LiCaAlF₆-Czochralski growth Authors (5): Zeng, Z; Chen, JQ ... Kawazoe, Y Published: May 2004 in Journal of Crystal Growth DOI: 10.1016/J.JCRYSGRO.2004.02.086</p>	9
<p>Thermodynamic properties of the Cu-Au system using a face-centered-cubic lattice model with a renormalized potential Published: May 2004 in The Journal of Chemical Physics DOI: 10.1063/1.1704633</p>	12
<p>First-principles study of the electronic structures of icosahedral TiN (N=13,19,43,55) clusters Authors (6): Wang, SY; Yu, JZ ... Wang, CY Published: May 2004 in The Journal of Chemical Physics DOI: 10.1063/1.1701769</p>	53
<p>Oscillatory thermocapillary convection in liquid bridge under microgravity Authors (5): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: May 2004 in Materials Transactions DOI: 10.2320/MATERTRANS.45.1522</p>	6
<p>Numerical study on LiCaAlF₆ Czochralski crystal growth Authors (8): Zeng, Z; Chen, JQ ... Kawazoe, Y Published: May 2004 in Materials Transactions DOI: 10.2320/MATERTRANS.45.1515</p>	3

Electronic transport properties of a metal-semiconductor carbon nanotube heterojunction Authors (3): Farajian, AA; Mizuseki, H; Kawazoe, Y Published: Apr 2004 in Physica E: Low-dimensional Systems and Nanostructures DOI: 10.1016/J.PHYSE.2003.12.097	17
Electronic structure and optical properties of the Co-doped anatase TiO ₂ studied from first principles Authors (6): Weng, HM; Yang, XP ... Kawazoe, Y Published: Mar 2004 in Physical Review B DOI: 10.1103/PHYSREVB.69.125219	159
Dynamical criteria for Cs ion insertion and adsorption at cap and stem of carbon nanotubes: Ab initio study and comparison with experiment Authors (7): Khazaei, M; Farajian, AA ... Kawazoe, Y Published: 2004 in The Journal of Physical Chemistry B DOI: 10.1021/JP0481557	23
Design proposal of light emitting diode in vacuum ultraviolet based on perovskite-like fluoride crystals Published: 2004 in JAPANESE JOURNAL OF APPLIED PHYSICS PART 2-LETTERS & EXPRESS LETTERS DOI: 10.1143/JJ.43.L1140	20
Electron transport in molecular enamel wires Authors (5): Belosludov, RV; Farajian, AA ... Kawazoe, Y Published: 2004 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.43.2061	14
Genetic algorithm approach to aromatic molecules for nanoscale device Authors (5): Mizuseki, H; Igarashi, N ... Kawazoe, Y Published: Dec 2003 in Materials Science and Engineering: C DOI: 10.1016/J.MSEC.2003.09.129	1
Cesium encapsulation in single-walled carbon nanotubes via plasma ion irradiation: Application to junction formation and ab initio investigation Authors (8): Jeong, GH; Farajian, AA ... Kawazoe, Y Published: Aug 2003 in Physical Review B DOI: 10.1103/PHYSREVB.68.075410	101
Ab initio study of divalent 3d transition metal impurities in KMgF ₃ and BaLiF ₃ Authors (8): Nishimatsu, T; Terakubo, N ... Fukuda, T Published: Aug 2003 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.42.5082	14
Encapsulation of cesium inside single-walled carbon nanotubes by plasma-ion irradiation method Authors (8): Jeong, GH; Farajian, AA ... Kawazoe, Y Published: Jul 2003 in Thin Solid Films DOI: 10.1016/S0040-6090(03)00337-7	39

<p>Molecular orbital analysis of frontier orbitals for molecular electronics: a case study of unimolecular rectifier and photovoltaic cell Authors (9): Mizuseki, Hiroshi; Belosludov, Rodion V. ... Kawazoe, Yoshiyuki Published: Jul 2003 in Science and Technology of Advanced Materials DOI: 10.1016/S1468-6996(03)00061-5</p>	10
<p>Low-energy surface collision induced dissociation of Ge and Sn cluster ions Authors (6): Tai, Y; Murakami, J ... Kawazoe, Y Published: Jun 2003 in The European Physical Journal D DOI: 10.1140/EPJD/E2003-00108-7</p>	14
<p>Thiophene thiol on the Au(111) surface: Size-dependent adsorption study Published: Jun 2003 in The Journal of Chemical Physics DOI: 10.1063/1.1560137</p>	25
<p>Electronic transport through bent carbon nanotubes: Nanoelectromechanical sensors and switches Authors (4): Farajian, AA; Yakobson, BI ... Kawazoe, Y Published: May 2003 in Physical Review B DOI: 10.1103/PHYSREVB.67.205423</p>	71
<p>Stability of Sb line structures on Si(001) Authors (7): Wang, JT; Mizuseki, H ... Wang, EG Published: May 2003 in Physical Review B DOI: 10.1103/PHYSREVB.67.193307</p>	19
<p>Three-dimensional oscillatory convection of LiCaAlF₆ melts in Czochralski crystal growth Authors (6): Zeng, Z; Chen, JQ ... Kawazoe, Y Published: May 2003 in Journal of Crystal Growth DOI: 10.1016/S0022-0248(03)00949-7</p>	27
<p>Control of substituent ligand over current through molecular devices: An ab initio molecular orbital theory Published: Mar 2003 in Physical Review B DOI: 10.1103/PHYSREVB.67.113408</p>	47
<p>Theoretical study of the alkyl derivative C₃₇H₅₀N₄O₄ molecule for use as a stable molecular rectifier: geometric and electronic structures Published: Mar 2003 in Computational Materials Science DOI: 10.1016/S0927-0256(02)00440-8</p>	17
<p>Theoretical study of donor-spacer-acceptor structure molecule for stable molecular rectifier Authors (7): Mizuseki, H; Niimura, K ... Majumder, C Published: Jan 2003 in Molecular Crystals and Liquid Crystals DOI: 10.1080/744818982</p>	30

Prediction of XPS spectra of silicon self-interstitials with the all-electron mixed-basis method Authors (7): Nishimatsu, T; Sluiter, M ... Uehara, M Published: 2003 in Physica B: Condensed Matter DOI: 10.1016/J.PHYSB.2003.09.133	6
Electronic transport through benzene molecule: effect of gold contacts Authors (4): Farajian, AA; Belosludov, RV ... Kawazoe, Y Published: 2003 in Physica E: Low-dimensional Systems and Nanostructures DOI: 10.1016/S1386-9477(02)01005-6	6
Theoretical study of phthalocyanine-fullerene complex for a high efficiency photovoltaic device using ab initio electronic structure calculation Authors (5): Mizuseki, H; Igarashi, N ... Kawazoe, Y Published: 2003 in Synthetic Metals DOI: 10.1016/S0379-6779(02)01289-4	34
Theoretical study of chlorin-fullerene supramolecular complexes for photovoltaic devices Authors (5): Mizuseki, H; Igarashi, N ... Kawazoe, Y Published: 2003 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.42.2503	18
Molecular enamel wires for electronic devices: Theoretical study Authors (6): Belosludov, RV; Sato, H ... Kawazoe, Y Published: 2003 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.42.2492	16
Theoretical study of molecular enamel wires based on polythiophene-cyclodextrin inclusion complexes Authors (5): Belosludov, RV; Sato, H ... Kawazoe, Y Published: 2003 in Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals DOI: 10.1080/15421400390263325	4
Theoretical study of insulated wires based on polymer chains encapsulated in molecular nanotubes Authors (5): Belosludov, RV; Sato, H ... Kawazoe, Y Published: 2003 in Thin Solid Films DOI: 10.1016/S0040-6090(03)00769-7	11
Theoretical study of donor-spacer-acceptor structure molecule for use as stable molecular rectifier: geometric and electronic structures Authors (6): Mizuseki, H; Igarashi, N ... Kawazoe, Y Published: 2003 in Thin Solid Films DOI: 10.1016/S0040-6090(03)00782-X	13

Marangoni Convection in the LiCaAlF(6) Crystal Growth by the Czochralski Technique Authors (6): Zeng, Zhong; Chen, Jingqiu ... Kawazoe, Yoshiyuki Published: Nov 2002 in Journal of Thermal Science DOI: 10.1007/S11630-002-0048-7	5
Interactions of a conjugated molecular diode with small metal clusters of Cu, Ag, and Au: First-principles calculations Published: Oct 2002 in The Journal of Chemical Physics DOI: 10.1063/1.1509053	38
Fragmentation of small tin cluster ions (Sn _x ⁺ : x=4-20) in the low-energy collisions with a highly oriented pyrolytic graphite surface Authors (6): Tai, Y; Murakami, J ... Kawazoe, Y Published: Sep 2002 in The Journal of Chemical Physics DOI: 10.1063/1.1496470	30
Structural investigation of thiophene thiol adsorption on Au nanoclusters: Influence of back bonds Published: Aug 2002 in The Journal of Chemical Physics DOI: 10.1063/1.1491404	61
Multiscale simulation of cluster growth and deposition processes by hybrid model based on direct simulation Monte Carlo method Authors (4): Mizuseki, H; Hongo, K ... Wille, LT Published: May 2002 in Computational Materials Science DOI: 10.1016/S0927-0256(02)00168-4	3
Theoretical Analysis for a Molecular Resonant Tunneling Diode Published: Apr 2002 in Japanese Journal of Applied Physics - Special Issues DOI: 10.1143/JJAP.41.2770	11
Theoretical study on inclusion complex of polyaniline covered by cyclodextrins for molecular device Authors (4): Belosludov, RV; Mizuseki, H ... Kawazoe, Y Published: Apr 2002 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.41.2739	30
Ionization potentials of small tin clusters: first principles calculations Authors (4): Majumder, C; Kumar, V ... Kawazoe, Y Published: Apr 2002 in Chemical Physics Letters DOI: 10.1016/S0009-2614(02)00333-0	18
Band structures of perovskite-like fluorides for vacuum-ultraviolet-transparent lens materials Authors (7): Nishimatsu, T; Terakubo, N ... Fukuda, T Published: Apr 2002 in Japanese Journal of Applied Physics DOI: 10.1143/JJAP.41.L365	125

<p>Hybrid model simulation of the cluster deposition process Authors (4): Hongo, K; Mizuseki, H ... Wille, LT Published: Mar 2002 in Journal of Crystal Growth DOI: 10.1016/S0022-0248(01)02106-6</p>	3
<p>Usefulness of experiments with model fluid for thermocapillary convection-effect of Prandtl number on two-dimensional thermocapillary convection Authors (6): Zeng, Z; Mizuseki, H ... Higashino, K Published: Jan 2002 in Journal of Crystal Growth DOI: 10.1016/S0022-0248(01)01700-6</p>	13
<p>Electron-interaction effects on transport characteristics of nanotubes Authors (4): Farajian, AA; Esfarjani, K ... Kawazoe, Y Published: 2002 in Physica B: Condensed Matter DOI: 10.1016/S0921-4526(02)00978-X</p>	1
<p>Simulation study on geometric and electronic structure of photovoltaic molecules Authors (8): Mizuseki, H; Igarashi, N ... Kawazoe, Y Published: 2002 in Materials Research Society Symposium - Proceedings DOI: 10.1557/PROC-725-P4.14</p>	6
<p>Molecular resistance in a molecular diode: A case study of the substituted phenylethynyl oligomer Authors (4): Majumder, C; Briere, T ... Kawazoe, Y Published: 2002 in The Journal of Physical Chemistry A DOI: 10.1021/JP0258560</p>	22
<p>Small clusters of tin: Atomic structures, energetics, and fragmentation behavior Authors (4): Majumder, C; Kumar, V ... Kawazoe, Y Published: Dec 2001 in Physical Review B DOI: 10.1103/PHYSREVB.64.233405</p>	87
<p>Structure similarity of mixed buoyancy-thermocapillary flow in half-zone liquid bridge Authors (6): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: Nov 2001 in Materials Transactions DOI: 10.2320/MATERTRANS.42.2322</p>	3
<p>Three-dimensional oscillatory thermocapillary convection in liquid bridge under microgravity Authors (6): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: Oct 2001 in International Journal of Heat and Mass Transfer DOI: 10.1016/S0017-9310(01)00012-6</p>	24
<p>Lattice Monte Carlo simulation with a renormalized potential in Si Published: Jul 2001 in Journal of Crystal Growth DOI: 10.1016/S0022-0248(01)01238-6</p>	4

<p>Marangoni convection in model of floating zone under microgravity Authors (6): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: Jul 2001 in Journal of Crystal Growth DOI: 10.1016/S0022-0248(01)01236-2</p>	25
<p>Multiscale simulation of cluster growth and deposition processes by direct simulation Monte Carlo method Authors (4): Mizuseki, H; Hongo, K ... Wille, LT Published: May 2001 in Scripta Materialia DOI: 10.1016/S1359-6462(01)00807-7</p>	5
<p>A Monte Carlo simulation on the process of cluster deposition Authors (3): Hongo, K; Mizuseki, H; Kawazoe, Y Published: Mar 2001 in Materials Transactions DOI: 10.2320/MATERTRANS.42.439</p>	5
<p>Molecular scale rectifier: Theoretical study Authors (3): Majumder, C; Mizuseki, H; Kawazoe, Y Published: 2001 in The Journal of Physical Chemistry A DOI: 10.1021/JP011888W</p>	54
<p>Direct Simulation Monte Carlo for Cluster Growth Process in Rarefied Gas Published: 2001 in Materials Transactions DOI: 10.2320/MATERTRANS.42.2295</p>	2
<p>Cluster growth processes by direct simulation Monte Carlo method Authors (4): Mizuseki, H; Jin, Y ... Wille, LT Published: 2001 in Applied Physics A DOI: 10.1007/S003390100911</p>	20
<p>Ab Initio Modeling of Real Molecular Logic Devices Published: 2001 in Materials Transactions DOI: 10.2320/MATERTRANS.42.2270</p>	4
<p>Bipyridinium Molecular Switch: Ab-initio Electronic Structure Calculation Published: 2001 in Materials Transactions DOI: 10.2320/MATERTRANS.42.2276</p>	4
<p>Growth processes of magnetic clusters studied by direct simulation Monte Carlo method Published: May 2000 in Journal of Applied Physics DOI: 10.1063/1.372770</p>	12
<p>Simulation of electrochemical deposition process by a multiparticle diffusive aggregation model Published: May 2000 in Journal of Applied Physics DOI: 10.1063/1.373110</p>	6

<p>A new crystal growth model based on a stochastic method under an external field Published: Jan 2000 in Modelling and Simulation in Materials Science and Engineering DOI: 10.1088/0965-0393/8/1/301</p>	7
<p>Weak Universality of a Site-Percolation Model with Two Different Sizes of Particles on a Square Lattice Published: Dec 1999 in Journal of the Physical Society of Japan DOI: 10.1143/JPSJ.68.3755</p>	12
<p>Marangoni convection in half-zone liquid bridge Authors (5): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: Nov 1999 in Materials Transactions DOI: 10.2320/MATERTRANS1989.40.1331</p>	6
<p>Direct numerical simulation of oscillatory Marangoni convection, in cylindrical liquid bridges Authors (4): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: Jul 1999 in Journal of Crystal Growth DOI: 10.1016/S0022-0248(99)00207-9</p>	26
<p>Body-centered-cubic lattice model with many-body interactions representing the melting transition in Si Published: May 1999 in The Journal of Chemical Physics DOI: 10.1063/1.478926</p>	11
<p>Numerical simulation of convection depth in shear cell under microgravity Authors (5): Zeng, Z; Mizuseki, H ... Kawazoe, Y Published: Jan 1999 in Advances in Space Research DOI: 10.1016/S0273-1177(99)00740-1</p>	3
<p>Simulation of Crystal Growth in Solution by Hybrid Modeling Published: 1999 in Materials Transactions, JIM DOI: 10.2320/MATERTRANS1989.40.1337</p>	1
<p>Site-Percolation Models Including Heterogeneous Particles on a Square Lattice Published: 1999 in Materials Transactions, JIM DOI: 10.2320/MATERTRANS1989.40.1314</p>	14
<p>Multi-valued magnetic recording materials predicted by self-organized magnetization dynamics Authors (4): Ishihara, M; Mizuseki, H ... Kawazoe, Y Published: 1999 in Materials Transactions DOI: 10.2320/MATERTRANS1989.40.1319</p>	1
<p>Monte Carlo Simulation of Cu&ndash;Au Alloys on FCC Lattice with a Renormalized Potential Published: 1999 in Materials Transactions, JIM DOI: 10.2320/MATERTRANS1989.40.911</p>	5

<p>Numerical study of dynamic behavior of melting sample in shear cell under microgravity</p> <p>Authors (5): Zeng, Z; Mizuseki, H ... Higashino, K</p> <p>Published: Nov 1998 in Numerical Heat Transfer, Part A: Applications</p> <p>DOI: 10.1080/10407789808914011</p>	9
<p>A new model of DLA under high magnetic field</p> <p>Published: Feb 1998 in Computational Materials Science</p> <p>DOI: 10.1016/S0927-0256(97)00142-0</p>	10
<p>Modelling of magnetic multivalued recording in granular material</p> <p>Authors (5): Mizuseki, H; Kikuchi, K ... Kawazoe, Y</p> <p>Published: 1998 in Japanese Journal of Applied Physics</p> <p>DOI: 10.1143/JJAP.37.2155</p>	2
<p>Unique magnetic properties of microclusters and their application to multi-valued magnetic recording media</p> <p>Authors (8): Kawazoe, Y; Li, ZQ ... Ohta, N</p> <p>Published: 1997 in Journal of the Korean Physical Society</p>	1
<p>A recording process simulation for double-layered magneto-optical disk</p> <p>Authors (4): Ishihara, M; Mizuseki, H ... Ohta, N</p> <p>Published: 1997 in IEEE Transactions on Magnetics</p> <p>DOI: 10.1109/20.619692</p>	1
<p>A new model for crystal growth under high magnetic field - Effect of environment in diffusion-limited aggregation</p> <p>Published: 1997 in Science Reports of the Research Institutes Tohoku University Series A-Physics Chemistry and Metallurgy</p>	6
<p>Short- and medium-range structure characteristics of amorphous alloys</p> <p>Authors (5): Suzuki, K; Fukunaga, T ... Mizuseki, H</p> <p>Published: 1997 in Thermodynamics of Alloy Formation</p>	16
<p>A Monte Carlo simulation describing melting transition of Si-type structure in the condensed phase with BCC lattice model including many-body interactions</p> <p>Published: 1997 in Science Reports of the Research Institutes Tohoku University Series A-Physics Chemistry and Metallurgy</p>	0
<p>Magnetic multi-valued recording by new magnetic configurations in 2D and 3D artificial lattices</p> <p>Authors (5): Mizuseki, H; Ishihara, M ... Ohta, N</p> <p>Published: 1996 in IEEE Transactions on Magnetics</p> <p>DOI: 10.1109/20.538861</p>	7
<p>Spin-reorientation transition in superlattices by large scale dynamic simulation</p> <p>Authors (5): Mizuseki, H; Ishihara, M ... Kawazoe, Y</p> <p>Published: 1996 in Materials Transactions</p> <p>DOI: 10.2320/MATERTRANS1989.37.478</p>	6

<p>Ultra-high density magnetic recording media using 2D and 3D magnetic anisotropic artificial lattices</p> <p>Authors (4): Mizuseki, H; Ishihara, M ... Kawazoe, Y</p> <p>Published: 1996 in Science Reports of the Research Institutes Tohoku University Series A-Physics Chemistry and Metallurgy</p>	3
<p>Dynamical properties of icosahedral quasicrystal and glassy Al₇₇Cu₁₃V₁₀: A comparative study by inelastic neutron scattering</p> <p>Published: Aug 1995 in Physica B: Condensed Matter</p> <p>DOI: 10.1016/0921-4526(95)00215-U</p>	2
<p>An interpretation of the low-energy excitations of Pd₇₉Ge₂₁ alloy glass within the soft-potential model</p> <p>Published: Aug 1995 in Physica B: Condensed Matter</p> <p>DOI: 10.1016/0921-4526(95)00204-M</p>	3
<p>AN OBSERVATION OF THE STRUCTURAL RELAXATION OF A Ni₄₀Pd₄₀P₂₀ AMORPHOUS ALLOY BY NEUTRON INELASTIC-SCATTERING</p> <p>Authors (5): OTOMO, T; ARAI, M ... SUZUKI, K</p> <p>Published: Aug 1995 in Physica B: Condensed Matter</p> <p>DOI: 10.1016/0921-4526(95)00206-O</p>	4
<p>The medium- and short-range collective atomic motion in Pd₇₅Si(Ge) amorphous alloys</p> <p>Authors (3): K. Suzuki; K. Shibata; H. Mizuseki</p> <p>Published: May 1993 in Journal of Non-Crystalline Solids</p> <p>DOI: 10.1016/0022-3093(93)90129-L</p>	25
<p>Correlated atomic motions in Pd₇₉Si₂₁ alloy glass observed by inelastic pulsed neutron scattering</p> <p>Authors (4): Kaoru Shibata; Hiroshi Mizuseki ... Kenji Suzuki</p> <p>Published: Nov 1992 in Journal of Non-Crystalline Solids</p> <p>DOI: 10.1016/0022-3093(92)90131-3</p>	6
<p>In situ observation of chemical vapour-deposited titanium oxide films by double-modulation infrared emission spectrometry</p> <p>Published: Dec 1991 in Vibrational Spectroscopy</p> <p>DOI: 10.1016/0924-2031(91)85031-H</p>	2