Susumu Yanagisawa

List of Publications by Year
in descending order

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67 papers	3,236 citations	361413 20 h-index	144013 57 g-index
67 all docs	67 docs citations	67 times ranked	4315 citing authors

#	Article	IF	Citations
1	Phonon dispersion of the organic semiconductor rubrene. Physical Review B, 2022, 105, .	3.2	5
2	Quantitative analysis of the electrostatic and electronic polarization energies in molecularly mixed films of organic semiconductors. Physical Review B, 2020, 102, .	3.2	6
3	Density Functional Theory-Based Molecular Modeling: Verification of Decisive Roles of Van der Waals Aggregation of Triiodide Ions for Effective Electron Transfer in Wet-Type N3-Dye-Sensitized Solar Cells. Energies, 2020, 13, 3027.	3.1	6
4	Nanoscale First-Principles Electronic Structure Simulations of Materials Relevant to Organic Electronics. , 2020, , 89-131.		1
5	Determination of the ionization energy and the electron affinity of organic molecular crystals from first-principles: dependence on the molecular orientation at the surface. Japanese Journal of Applied Physics, 2020, 59, 031002.	1.5	3
6	Quantum chemistry molecular modelling for mitochondria targeted chemotherapy: Verification of oxidative stress on mitochondria and anticancer medicines. Integrative Molecular Medicine, 2020, 7, .	0.3	1
7	Enhancement of the GW Space-Time Program Code for Accurate Prediction of the Electronic Properties of Organic Electronics Materials. , 2020, , 225-234.		0
8	Experimental and computational studies on ruthenium(<scp>ii</scp>) bis-diimine complexes of N,Nâ€²-chelate ligands: the origin of changes in absorption spectra upon oxidation and reduction. Physical Chemistry Chemical Physics, 2019, 21, 7973-7988.	2.8	9
9	A New Pentacene Polymorph Induced by Interaction with a Bi(0001) Substrate. Journal of Physical Chemistry C, 2018, 122, 6240-6245.	3.1	4
10	Validity of density-functional-theory-based molecular modeling for UV/visible spectroscopy and rationale of panchromatic PbI6 4â^'(MeNH3 +)4-structured molecular solar cells. Japanese Journal of Applied Physics, 2018, 57, 121602.	1.5	1
11	Surface Structure of Organic Semiconductor [n]Phenacene Single Crystals. Journal of the American Chemical Society, 2018, 140, 14046-14049.	13.7	5
12	Impact of the molecular quadrupole moment on ionization energy and electron affinity of organic thin films: Experimental determination of electrostatic potential and electronic polarization energies. Physical Review B, 2018, 97, .	3.2	47
13	Determination of geometric and electronic structures of organic crystals from first principles: Role of the molecular configuration on the electronic structure. Journal of Applied Physics, 2017, 121, 045501.	2.5	14
14	First-Principles Molecular Dynamics Analysis of Ligand-Free Suzukiâ€“Miyaura Cross-Coupling in Water Solvent: Oxidative Addition Step. Journal of Physical Chemistry B, 2017, 121, 164-173.	2.6	10
15	Augmented pH-sensitivity absorbance of a ruthenium(<scp>ii</scp>) bis(bipyridine) complex with elongation of the conjugated ligands: an experimental and theoretical investigation. Physical Chemistry Chemical Physics, 2017, 19, 25734-25745.	2.8	6
16	First-Principles Molecular Dynamics Analysis of Ligand-Free Suzukiâ€“Miyaura Cross-Coupling in Water: Transmetalation and Reductive Elimination. Journal of Physical Chemistry C, 2017, 121, 19904-19914.	3.1	9
17	Computational Verification of So-Called Perovskite Solar Cells as PbI₆^{4â^'}-Aligned Solar Cells. Journal of the Electrochemical Society, 2017, 164, E3598-E3605.	2.9	3
18	Theoretical determination of the ionization potential and the electron affinity of organic semiconductors. AIP Conference Proceedings, 2017, , .	0.4	3

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19	Molecular-Orbital-Based Verification of Water Photo-Splitting on Pt-Loaded TiO2: Effective Formation of HOOH and Reduced Platinum Cluster as Precursors of O2and H2. ECS Transactions, 2017, 80, 1091-1112.	0.5	1
20	Theoretical Study on Electronic Structure of Bathocuproine: Renormalization of the Band Gap in the Crystalline State and the Large Exciton Binding Energy. Journal of the Chinese Chemical Society, 2016, 63, 513-520.	1.4	2
21	Charge transfer states appear in the Ï€-conjugated pure hydrocarbon molecule on Cu(111). Applied Physics Express, 2016, 9, 045201.	2.4	10
22	Suppressing molecular vibrations in organic semiconductors by inducing strain. Nature Communications, 2016, 7, 11156.	12.8	105
23	Tensile-strain effect of inducing the indirect-to-direct band-gap transition and reducing the band-gap energy of Ge. Journal of Applied Physics, 2015, 118, 105704.	2.5	13
24	Theoretical Verification of Photoelectrochemical Water Oxidation Using Nanocrystalline TiO2 Electrodes. Molecules, 2015, 20, 9732-9744.	3.8	4
25	Recent progress in predicting structural and electronic properties of organic solids with the van der Waals density functional. Journal of Electron Spectroscopy and Related Phenomena, 2015, 204, 159-167.	1.7	10
26	Molecular Orbital-Based Verification of Conductivity of Tetramethylammonium Pentaiodide and Pentaiodide-Based Electrolytes in Dye-Sensitized Solar Cells. Journal of the Electrochemical Society, 2015, 162, E263-E270.	2.9	8
27	Publisher's Note: Origin of the band dispersion in a metal phthalocyanine crystal [Phys. Rev. B90, 245141 (2014)]. Physical Review B, 2015, 91, .	3.2	0
28	Origin of the band dispersion in a metal phthalocyanine crystal. Physical Review B, 2014, 90, .	3.2	15
29	Scanning tunneling microscopy/spectroscopy of picene thin films formed on Ag(111). Journal of Chemical Physics, 2014, 141, 114701.	3.0	21
30	Search for a Self-Regenerating Perovskite Catalyst with Ab Initio Thermodynamics II: Cu-Doped Layered Perovskites with K2NiF4 Structure. Catalysis Letters, 2014, 144, 736-743.	2.6	6
31	Theoretical investigation of the band structure of picene single crystals within the GW approximation. Japanese Journal of Applied Physics, 2014, 53, 05FY02.	1.5	13
32	Internal-strain effect on the valence band of strained silicon and its correlation with the bond angles. Journal of Applied Physics, 2014, 115, .	2.5	1
33	Intermolecular Interaction as the Origin of Red Shifts in Absorption Spectra of Zinc-Phthalocyanine from First-Principles. Journal of Physical Chemistry A, 2013, 117, 11246-11253.	2.5	37
34	First-principles investigation on the segregation of Pd at LaFe1-xPd x O3-y surfaces. Nanoscale Research Letters, 2013, 8, 203.	5.7	25
35	HOMO band dispersion of crystalline rubrene: Effects of self-energy corrections within theGWapproximation. Physical Review B, 2013, 88, .	3.2	38
36	Search for a Self-Regenerating Perovskite Catalyst Using ab Initio Thermodynamics Calculations. Journal of Physical Chemistry C, 2013, 117, 1278-1286.	3.1	30

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37	Anisotropy of the silicon valence band induced by strain with various orientations. Journal of Applied Physics, 2013, 113, .	2.5	4
38	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. Current Applied Physics, 2012, 12, S2-S9.	2.4	18
39	Local electronic properties at organicâ€“metal interfaces: thiophene derivatives on Pt(111). Physical Chemistry Chemical Physics, 2012, 14, 15412.	2.8	9
40	Density Functional Theoretical Study of Perfluoropentacene/Noble Metal Interfaces with van der Waals Corrections: Adsorption States and Vacuum Level Shifts. Journal of Physical Chemistry C, 2011, 115, 5767-5772.	3.1	23
41	First-principles Theoretical Study of Organic-metal Interfaces. Hyomen Kagaku, 2011, 32, 9-14.	0.0	1
42	Density-functional theoretical study of fluorination effect on organic/metal interfaces. Organic Electronics, 2011, 12, 295-299.	2.6	13
43	Adsorption of Benzene on Noble Metal Surfaces Studied by Density Functional Theory with Van der Waals Correction. Journal of Nanoscience and Nanotechnology, 2011, 11, 2836-2843.	0.9	11
44	Adsorption of Alq<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>on Mg(001) surface: Role of chemical bonding, molecular distortion, and van der Waals interaction. Physical Review B, 2011, 83, .	3.2	7
45	Pseudopotential approximation in van der Waals density functional calculations. Physical Review B, 2011, 84, .	3.2	20
46	Origin of Surface-Band Dispersion at the Pentacene/Cu Interface. Applied Physics Express, 2010, 3, 025701.	2.4	9
47	State-selective dissociation of a single water molecule on an ultrathin MgO film. Nature Materials, 2010, 9, 442-447.	27.5	171
48	C₆₀ Adsorbed on Platinum Surface: A Good Mediator of Metal Wave Function. Journal of Physical Chemistry C, 2010, 114, 3504-3506.	3.1	20
49	Density functional theoretical study of pentacene/noble metal interfaces with van der Waals corrections: Vacuum level shifts and electronic structures. Journal of Chemical Physics, 2010, 132, 134703.	3.0	118
50	First-principles study of the pentacene/Cu(111) interface: Adsorption states and vacuum level shifts. Journal of Electron Spectroscopy and Related Phenomena, 2009, 174, 78-84.	1.7	45
51	First-principles study of benzene on noble metal surfaces: Adsorption states and vacuum level shifts. Surface Science, 2009, 603, 2912-2922.	1.9	82
52	Organic/Metal Interfaces: From Elementary Electronic Structure to Organic Electronic Devices. Journal of Computational and Theoretical Nanoscience, 2009, 6, 2499-2513.	0.4	2
53	Theoretical investigation of the electronic structure of the Alq₃Mg interface. Journal of Physics Condensed Matter, 2009, 21, 064247.	1.8	12
54	Theoretical study of vacuum level shift at the C₆H₆/Al(111) interface. Surface and Interface Analysis, 2008, 40, 1059-1062.	1.8	8

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55	Role of Molecular Orbitals Near the Fermi Level in the Excitation of Vibrational Modes of a Single Molecule at a Scanning Tunneling Microscope Junction. Physical Review Letters, 2008, 100, 136104.	7.8	71
56	First-principles theoretical study of Alq3âˆ•Al interfaces: Origin of the interfacial dipole. Journal of Chemical Physics, 2008, 128, 244704.	3.0	51
57	A first-principles investigation on the mechanism of nitrogen dissolution in the Na flux method. Journal of Applied Physics, 2007, 101, 066106.	2.5	11
58	A first-principles study on nitrogen solubility in Na flux toward theoretical search for a novel flux for bulk GaN growth. Journal of Crystal Growth, 2007, 303, 34-36.	1.5	15
59	First-principles molecular dynamics study of Al/Alq3interfaces. Science and Technology of Advanced Materials, 2007, 8, 191-195.	6.1	11
60	Important role of molecular permanent dipoles of the Alq3/Al interface studied from first-principles. Chemical Physics Letters, 2006, 420, 523-528.	2.6	39
61	Theoretical Investigation on the Electronic Structure of the Tris-(8-hydroxyquinolinato) Aluminum/Aluminum Interface. Japanese Journal of Applied Physics, 2006, 45, 413-416.	1.5	18
62	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. Computational and Theoretical Chemistry, 2005, 716, 45-60.	1.5	22
63	INVESTIGATION OF DOMINANT ELECTRON CONFIGURATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. Journal of Theoretical and Computational Chemistry, 2005, 04, 265-280.	1.8	2
64	A long-range-corrected time-dependent density functional theory. Journal of Chemical Physics, 2004, 120, 8425-8433.	3.0	1,694
65	Investigation of the use of density functionals in second- and third-row transition metal dimer calculations. Journal of Computational Chemistry, 2001, 22, 1995-2009.	3.3	39
66	The relativistic effect on energies of light elements: a RESC-BOP study. Computational and Theoretical Chemistry, 2001, 537, 63-70.	1.5	10
67	An investigation of density functionals: The first-row transition metal dimer calculations. Journal of Chemical Physics, 2000, 112, 545-553.	3.0	208