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	A long-range-corrected time-dependent density functional theory. Journal of Chemical Physics, 2004, 120, 8425-8433.	3.0	1,694
2	An investigation of density functionals: The first-row transition metal dimer calculations. Journal of Chemical Physics, 2000, 112, 545-553.	3.0	208
3	State-selective dissociation of a single water molecule on an ultrathin MgO film. Nature Materials, 2010, 9, 442-447.	27.5	171
4	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
5	Suppressing molecular vibrations in organic semiconductors by inducing strain. Nature Communications, 2016, 7, 11156.	12.8	105
6	First-principles study of benzene on noble metal surfaces: Adsorption states and vacuum level shifts. Surface Science, 2009, 603, 2912-2922.	1.9	82
7	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
8	First-principles theoretical study of Alq3â^•Al interfaces: Origin of the interfacial dipole. Journal of Chemical Physics, 2008, 128, 244704.	3.0	51
9	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
10	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
11	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
12	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
13	HOMO band dispersion of crystalline rubrene: Effects of self-energy corrections within theGWapproximation. Physical Review B, 2013, 88, .	3.2	38
14	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
15	Search for a Self-Regenerating Perovskite Catalyst Using ab Initio Thermodynamics Calculations. Journal of Physical Chemistry C, 2013, 117, 1278-1286.	3.1	30
16	First-principles investigation on the segregation of Pd at LaFe1-xPd x O3-y surfaces. Nanoscale Research Letters, 2013, 8, 203.	5.7	25
17	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
18	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. Computational and Theoretical Chemistry, 2005, 716, 45-60.	1.5	22

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19	Scanning tunneling microscopy/spectroscopy of picene thin films formed on Ag(111). Journal of Chemical Physics, 2014, 141, 114701.	3.0	21
20	C₆₀ Adsorbed on Platinum Surface: A Good Mediator of Metal Wave Function. Journal of Physical Chemistry C, 2010, 114, 3504-3506.	3.1	20
21	Pseudopotential approximation in van der Waals density functional calculations. Physical Review B, 2011, 84, .	3.2	20
22	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
23	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. Current Applied Physics, 2012, 12, S2-S9.	2.4	18
24	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
25	Origin of the band dispersion in a metal phthalocyanine crystal. Physical Review B, 2014, 90, .	3.2	15
26	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
27	Density-functional theoretical study of fluorination effect on organic/metal interfaces. Organic Electronics, 2011, 12, 295-299.	2.6	13
28	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
29	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
30	Theoretical investigation of the electronic structure of the Alq₃Mg interface. Journal of Physics Condensed Matter, 2009, 21, 064247.	1.8	12
31	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
32	First-principles molecular dynamics study of Al/Alq3interfaces. Science and Technology of Advanced Materials, 2007, 8, 191-195.	6.1	11
33	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
34	The relativistic effect on energies of light elements: a RESC-BOP study. Computational and Theoretical Chemistry, 2001, 537, 63-70.	1.5	10
35	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
36	Charge transfer states appear in the Ï€-conjugated pure hydrocarbon molecule on Cu(111). Applied Physics Express, 2016, 9, 045201.	2.4	10

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37	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
38	Origin of Surface-Band Dispersion at the Pentacene/Cu Interface. Applied Physics Express, 2010, 3, 025701.	2.4	9
39	Local electronic properties at organicâ€“metal interfaces: thiophene derivatives on Pt(111). Physical Chemistry Chemical Physics, 2012, 14, 15412.	2.8	9
40	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
41	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
42	Theoretical study of vacuum level shift at the C₆H₆/Al(111) interface. Surface and Interface Analysis, 2008, 40, 1059-1062.	1.8	8
43	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
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	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
46	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
47	Quantitative analysis of the electrostatic and electronic polarization energies in molecularly mixed films of organic semiconductors. Physical Review B, 2020, 102, .	3.2	6
48	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
49	Surface Structure of Organic Semiconductor [n]Phenacene Single Crystals. Journal of the American Chemical Society, 2018, 140, 14046-14049.	13.7	5
50	Phonon dispersion of the organic semiconductor rubrene. Physical Review B, 2022, 105, .	3.2	5
51	Anisotropy of the silicon valence band induced by strain with various orientations. Journal of Applied Physics, 2013, 113, .	2.5	4
52	Theoretical Verification of Photoelectrochemical Water Oxidation Using Nanocrystalline TiO2 Electrodes. Molecules, 2015, 20, 9732-9744.	3.8	4
53	A New Pentacene Polymorph Induced by Interaction with a Bi(0001) Substrate. Journal of Physical Chemistry C, 2018, 122, 6240-6245.	3.1	4
54	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

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55	Theoretical determination of the ionization potential and the electron affinity of organic semiconductors. AIP Conference Proceedings, 2017, , .	0.4	3
56	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
57	INVESTIGATION OF DOMINANT ELECTRON CONFIGURATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. Journal of Theoretical and Computational Chemistry, 2005, 04, 265-280.	1.8	2
58	Organic/Metal Interfaces: From Elementary Electronic Structure to Organic Electronic Devices. Journal of Computational and Theoretical Nanoscience, 2009, 6, 2499-2513.	0.4	2
59	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
60	First-principles Theoretical Study of Organic-metal Interfaces. Hyomen Kagaku, 2011, 32, 9-14.	0.0	1
61	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
62	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
63	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
64	Nanoscale First-Principles Electronic Structure Simulations of Materials Relevant to Organic Electronics. , 2020, , 89-131.		1
65	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
66	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
67	Enhancement of the GW Space-Time Program Code for Accurate Prediction of the Electronic Properties of Organic Electronics Materials. , 2020, , 225-234.		0