Tiem Leong Yoon

List of Publications by Year
in descending order

75	619	566801 15	713013 21
papers	citations	h-index	g-index

77	77	77	773
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effects of Hubbard term correction on the structural parameters and electronic properties of wurtzite ZnO. Computational Materials Science, 2017, 138, 111-116.	1.4	55
2	Mechanical and electronic properties of graphitic carbon nitride sheet: First-principles calculations. Solid State Communications, 2016, 248, 144-150.	0.9	35
3	First-principles studies on the superconductivity of aluminene. Applied Surface Science, 2018, 445, 161-166.	3.1	28
4	Surface and interface phonon polaritons of wurtzite GaN thin film grown on 6H-SiC substrate. Applied Physics Letters, 2009, 94, .	1.5	26
5	AERONET dataâ€“based determination of aerosol types. Atmospheric Pollution Research, 2015, 6, 682-695.	1.8	25
6	First-principles study of monolayer Be2C as an anode material for lithium-ion batteries. Journal of Applied Physics, 2019, 126, .	1.1	23
7	Studying the varied shapes of gold clusters by an elegant optimization algorithm that hybridizes the density functional tight-binding theory and the density functional theory. Computer Physics Communications, 2017, 220, 143-149.	3.0	21
8	First-principles investigation of graphitic carbon nitride monolayer with embedded Fe atom. Surface Science, 2018, 667, 112-120.	0.8	20
9	Geometric and electric properties of graphitic carbon nitride sheet with embedded single manganese atom under bi-axial tensile strain. Current Applied Physics, 2016, 16, 809-815.	1.1	19
10	Molecular dynamics simulation of thermodynamic and thermal transport properties of strontium titanate with improved potential parameters. Computational Materials Science, 2012, 60, 123-129.	1.4	18
11	Strain-tunable electronic and magnetic properties of two-dimensional gallium nitride with vacancy defects. Journal of Applied Physics, 2020, 127, .	1.1	18
12	Comparison of FTIR spectrum with chemometric and machine learning classifying analysis for differentiating guan-mutong a nephrotoxic and carcinogenic traditional chinese medicine with chuan-mutong. Microchemical Journal, 2021, 163, 105835.	2.3	17
13	Effects of nitrogen addition and growth condition on the enhanced mechanical properties of transition metal carbides TMC (TM = Zr, Hf). Ceramics International, 2020, 46, 1124-1136.	2.3	16
14	Metal-free ferromagnetic semiconductor: Mechanical, electronic and magnetic properties of boron doped graphitic carbon nitride (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	2.0	16
15	Integrated <scp>SnSSe</scp> bulk and monolayer as industrial waste heat thermoelectric materials. International Journal of Energy Research, 2021, 45, 2085-2099.	2.2	16
16	X-ray diffraction experiments, luminescence measurements and first-principles GGA+U calculations on YTaO4. Computational Materials Science, 2013, 77, 13-18.	1.4	15
17	Epitaxial growth of graphene on 6H-silicon carbide substrate by simulated annealing method. Journal of Chemical Physics, 2013, 139, 204702.	1.2	15
18	Effect of chemical interface damping and aggregation size of bare gold nanoparticles in NaCl on the plasmon resonance damping. Optical Materials Express, 2017, 7, 955.	1.6	15

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19	Monsoonal variations in aerosol optical properties and estimation of aerosol optical depth using ground-based meteorological and air quality data in Peninsular Malaysia. Atmospheric Chemistry and Physics, 2015, 15, 3755-3771.	1.9	14
20	Theoretical studies on mechanical and electronic properties of s-triazine sheet. Philosophical Magazine, 2017, 97, 2077-2088.	0.7	13
21	First-principles studies on the effects of halogen adsorption on monolayer antimony. Physical Chemistry Chemical Physics, 2017, 19, 25786-25795.	1.3	13
22	Structural and response properties of all BaTiO3 phases from density functional theory using the projector-augmented-wave methods. Computational Materials Science, 2016, 117, 306-314.	1.4	11
23	Monolayer GaN functionalized with alkali metal and alkaline earth metal atoms: A first-principles study. Superlattices and Microstructures, 2019, 130, 428-436.	1.4	11
24	Effects of atoms and molecules adsorption on electronic and magnetic properties of s-triazine with embedded Fe atom: DFT investigations. Philosophical Magazine, 2018, 98, 1114-1129.	0.7	10
25	Molecular dynamics simulation of melting of silicene. Materials Research Express, 2018, 5, 065054.	0.8	10
26	Frequency dependent linear and nonlinear optical properties of compositionally tuned inorganic CsSnX (XÂ= Br, I) composites. Journal of Alloys and Compounds, 2019, 779, 497-504.	2.8	10
27	A first-principles study of two-dimensional NbSe₂H/g-ZnO van der Waals heterostructures as a water splitting photocatalyst. Physical Chemistry Chemical Physics, 2021, 23, 24222-24232.	1.3	10
28	High-pressure phases of AlxIn1â^'xN compounds: First principles calculations. Journal of Alloys and Compounds, 2017, 704, 160-169.	2.8	9
29	Ab initio computations of the linear and nonlinear optical properties of stable compounds in AlInN system. Current Applied Physics, 2016, 16, 1277-1283.	1.1	8
30	A molecular dynamics study of the thermodynamic properties of barium zirconate. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 045001.	0.8	6
31	Structural relaxation of BaTiO3 slab with tetragonal (100) surface: Ab-initio comparison of different thickness. Current Applied Physics, 2016, 16, 1491-1497.	1.1	6
32	Selective hydrogen adsorption on a buckled carbon nitride sheet: first-principles calculation. Materials Research Express, 2018, 5, 125605.	0.8	6
33	Elastic and electronic properties of C₂N monolayer: first-principles calculation. Materials Research Express, 2019, 6, 025601.	0.8	6
34	The development of a multigroup Monte Carlo code for TRIGA reactors. Nuclear Engineering and Design, 2019, 342, 99-114.	0.8	5
35	Metal to semiconductor transition of two-dimensional NbSe2 through hydrogen adsorption: A first-principles study. Journal of Applied Physics, 2020, 128, 105301.	1.1	5
36	Molecular dynamics simulations and photoluminescence measurements of annealed ZnO surfaces. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 90, 28-36.	1.3	4

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37	Thermoelectric and piezoelectric properties of the predicted Al_xIn_{1â^'x}N composites based on ab initio calculations. Physical Chemistry Chemical Physics, 2017, 19, 24613-24625.	1.3	4
38	Biogas detection on carbon nitride sheet with embedded Mn atom: dispersion-corrected density functional theory. Materials Research Express, 2019, 6, 065603.	0.8	4
39	Tuning the electronic and magnetic properties of Fe atom embedded heptazine sheet by atomic and molecular adsorption: First-principles calculations. Chinese Journal of Physics, 2019, 57, 1-5.	2.0	4
40	An efficient Monte Carlo fission source convergence acceleration strategy adapted from the survival biasing technique. Annals of Nuclear Energy, 2020, 138, 107164.	0.9	4
41	A novel machine learning scheme for classification of medicinal herbs based on 2D-FTIR fingerprints. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 266, 120440.	2.0	4
42	Maximal Î½Î¼â€“Î½Ï„ oscillations, the see-saw mechanism and the Exact Parity Model. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 2000, 491, 291-296.	1.5	3
43	Thorough investigations of the structural and electronic properties of AlxIn1-xN ternary compound via ab initio computations. Journal of Alloys and Compounds, 2016, 682, 338-344.	2.8	3
44	Functionalization of single-layer Pmma-CO by adatoms: A first-principles study of electronic, magnetic and structural properties. Journal of Physics and Chemistry of Solids, 2018, 123, 294-299.	1.9	3
45	Effects of oxygen variation on the improved structural stability, electronic and optical properties of ZnTeO compounds. Journal of Physics Condensed Matter, 2020, 32, 225701.	0.7	3
46	Resonance position and extinction efficiency of a single silica coated gold nanoshell when size effects of core is matter. AIP Conference Proceedings, 2017, , .	0.3	3
47	Solutions of the atmospheric, solar, and LSND neutrino anomalies from TeV scale quark-lepton unification. Physical Review D, 2001, 65, .	1.6	2
48	Multiple regression method to determine aerosol optical depth in atmospheric column in Penang, Malaysia. IOP Conference Series: Earth and Environmental Science, 2014, 18, 012081.	0.2	2
49	Ground-state structures of Hafnium clusters. AIP Conference Proceedings, 2015, , .	0.3	2
50	DFTB parameterization and its application for the global minimum search of the small boron-carbon clusters. Chemical Physics Letters, 2019, 716, 207-210.	1.2	2
51	The generation of groundâ€state structures and electronic properties of ternary Al k Ti l Ni m clusters (k â€‰+â€‰ l â€‰+â€‰ m â€‰=â€‰4) from a twoâ€stage density functional theory global searching approach. International Journal of Quantum Chemistry, 2019, 119, e25884.	1.0	2
52	Magnetic resonance imaging (MRI) compatible ZrX (Xâ€¯=â€¯Hf, Mo and Ru) alloys with enhanced mechanical properties as alternative biomedical applications. Scripta Materialia, 2020, 178, 82-85.	2.6	2
53	Electronics and magnetic properties of p-block elements doped 2D buckled gallium nitride MGaN (M =) Tj ETQq1 1 0.784314 rgBT /Ov	0.3	2
54	A polynomial model of transmission and reflection of electromagnetic monochromatic plane waves in lossless, non-magnetic multilayer thin films subjected to an external transverse voltage. Optical and Quantum Electronics, 2021, 53, 1.	1.5	2

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55	Mechanical and optical properties of polymeric nitrogen achieved by compression: DFT study. Materialia, 2021, 20, 101206.	1.3	2
56	Adsorption and decomposition of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si14.svg"><mml:mrow><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="bold">S</mml:mi></mml:mrow></mml:math> on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si15.svg"><mml:mrow><mml:msub><mml:mi mathvariant="bold">C</mml:mi><mml:mn>2</mml:mn></mml:msub>	0.9	2
57	Molecular dynamics study of thermal expansion and isothermal compressibility of strontium titanate and barium zirconate. , 2013, , .		1
58	Magnetic Moments due to Orbital Currents in an Electron-Lattice Model of Cuprate Superconductors. Journal of Superconductivity and Novel Magnetism, 2014, 27, 2673-2677.	0.8	1
59	Manipulating API and AOD data to distinguish transportation of aerosol at high altitude in Penang, Malaysia. IOP Conference Series: Earth and Environmental Science, 2014, 18, 012082.	0.2	1
60	Guided basin-hopping search of small boron clusters with density functional theory. AIP Conference Proceedings, 2015, , .	0.3	1
61	Molecular dynamics simulation of annealed ZnO surfaces. AIP Conference Proceedings, 2015, , .	0.3	1
62	Growth of bi- and tri-layered graphene on silicon carbide substrate via molecular dynamics simulation. AIP Conference Proceedings, 2015, , .	0.3	1
63	Investigation of Melting Dynamics of Hafnium Clusters. Journal of Chemical Information and Modeling, 2017, 57, 517-528.	2.5	1
64	Theory of d-Wave High Temperature Superconductivity in the Cuprates Involving Non-linear Lattice Modes. Journal of Superconductivity and Novel Magnetism, 2017, 30, 3377-3395.	0.8	1
65	Halogenated monolayer SnS: a first-principles studies. IOP Conference Series: Materials Science and Engineering, 2019, 625, 012001.	0.3	1
66	Calculation of ground state energy of a â€œ4 Ã— 4â€•flux qubit Josephson junction array using diffusion quantum Monte Carlo method. , 2013, , .		0
67	Influence of force constant on surface phonon polariton properties of cubic ZnS1â^'xSex crystals. AIP Conference Proceedings, 2015, , .	0.3	0
68	Electronic and magnetic properties of small rhodium clusters. AIP Conference Proceedings, 2015, , .	0.3	0
69	Structures of 38-atom gold-platinum nanoalloy clusters. AIP Conference Proceedings, 2015, , .	0.3	0
70	Melting behaviour of gold-platinum nanoalloy clusters by molecular dynamics simulations. AIP Conference Proceedings, 2015, , .	0.3	0
71	Structural properties of small rhodium clusters. AIP Conference Proceedings, 2015, , .	0.3	0
72	Hydrogen bond sensing ability of CdSe/ZnS colloidal quantum dots in ionic medium. Materials Research Express, 2019, 6, 015016.	0.8	0

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73	Generation of groundâ€state structures and electronic properties of ternary Al x Ti y Ni z clusters (x â€‰+â€‰) Tj ETQq1 1 0.784314 r Quantum Chemistry, 2020, 120, e26079.	1.0	0
74	Pressureâ€induced enhancement of mechanical performance in ZrC system. International Journal of Quantum Chemistry, 0, , .	1.0	0
75	New phase of lead chalcogenide alloy: Ternary alloy PbSrSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math> for future thermoelectric application. Materialia, 2022, 23, 101443.	1.3	0