## Tiem Leong Yoon

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

67	415	12	16
papers	citations	h-index	g-index
77	520	3	4.17
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
67	Adsorption and decomposition of H2S on C2N sheet with embedded manganese atom: First-principles calculations. <i>Chemical Physics</i> , <b>2022</b> , 555, 111443	2.3	O
66	A novel machine learning scheme for classification of medicinal herbs based on 2D-FTIR fingerprints. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2022</b> , 266, 120440	4.4	1
65	New phase of lead chalcogenide alloy: Ternary alloy PbSrSe2 for future thermoelectric application. <i>Materialia</i> , <b>2022</b> , 23, 101443	3.2	
64	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. <i>Microchemical Journal</i> , <b>2021</b> , 163, 105835	4.8	5
63	Integrated SnSSe bulk and monolayer as industrial waste heat thermoelectric materials.  International Journal of Energy Research, 2021, 45, 2085-2099	4.5	5
62	Electronics and magnetic properties of p-block elements doped 2D buckled gallium nitride MGaN (M = Al, Si, P and S): A first-principles study <b>2021</b> ,		1
61	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. <i>Optical and Quantum Electronics</i> , <b>2021</b> , 53, 1	2.4	O
60	Mechanical and optical properties of polymeric nitrogen achieved by compression: DFT study. <i>Materialia</i> , <b>2021</b> , 20, 101206	3.2	1
59	A first-principles study of two-dimensional NbSeH/g-ZnO van der Waals heterostructures as a water splitting photocatalyst. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 24222-24232	3.6	O
58	Metal-free ferromagnetic semiconductor: Mechanical, electronic and magnetic properties of boron doped graphitic carbon nitride (gtt6N6) sheet. <i>Materials Chemistry and Physics</i> , <b>2020</b> , 254, 123470	4.4	8
57	Magnetic resonance imaging (MRI) compatible ZrX (X = Hf, Mo and Ru) alloys with enhanced mechanical properties as alternative biomedical applications. <i>Scripta Materialia</i> , <b>2020</b> , 178, 82-85	5.6	1
56	Generation of ground-state structures and electronic properties of ternary AlxTiyNiz clusters ( $x + y + z = 6$ ) with a two-stage density functional theory global search approach. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26079	2.1	
55	An efficient Monte Carlo fission source convergence acceleration strategy adapted from the survival biasing technique. <i>Annals of Nuclear Energy</i> , <b>2020</b> , 138, 107164	1.7	4
54	Strain-tunable electronic and magnetic properties of two-dimensional gallium nitride with vacancy defects. <i>Journal of Applied Physics</i> , <b>2020</b> , 127, 015305	2.5	8
53	Metal to semiconductor transition of two-dimensional NbSe2 through hydrogen adsorption: A first-principles study. <i>Journal of Applied Physics</i> , <b>2020</b> , 128, 105301	2.5	1
52	Effects of nitrogen addition and growth condition on the enhanced mechanical properties of transition metal carbides TMC (TM = Zr, Hf). <i>Ceramics International</i> , <b>2020</b> , 46, 1124-1136	5.1	9
51	Effects of oxygen variation on the improved structural stability, electronic and optical properties of ZnTeO compounds. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 225701	1.8	1

## (2017-2019)

50	First-principles study of monolayer Be2C as an anode material for lithium-ion batteries. <i>Journal of Applied Physics</i> , <b>2019</b> , 126, 125302	2.5	12
49	Monolayer GaN functionalized with alkali metal and alkaline earth metal atoms: A first-principles study. Superlattices and Microstructures, <b>2019</b> , 130, 428-436	2.8	7
48	Biogas detection on carbon nitride sheet with embedded Mn atom: dispersion-corrected density functional theory. <i>Materials Research Express</i> , <b>2019</b> , 6, 065603	1.7	3
47	Halogenated monolayer SnS: a first-principles studies. <i>IOP Conference Series: Materials Science and Engineering</i> , <b>2019</b> , 625, 012001	0.4	1
46	DFTB parameterization and its application for the global minimum search of the small boron-carbon clusters. <i>Chemical Physics Letters</i> , <b>2019</b> , 716, 207-210	2.5	1
45	The development of a multigroup Monte Carlo code for TRIGA reactors. <i>Nuclear Engineering and Design</i> , <b>2019</b> , 342, 99-114	1.8	3
44	The generation of ground-state structures and electronic properties of ternary AlkTilNim clusters $(k + l + m = 4)$ from a two-stage density functional theory global searching approach. <i>International Journal of Quantum Chemistry</i> , <b>2019</b> , 119, e25884	2.1	1
43	Frequency dependent linear and nonlinear optical properties of compositionally tuned inorganic CsSnX (X = Br, I) composites. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 779, 497-504	5.7	5
42	Tuning the electronic and magnetic properties of Fe atom embedded heptazine sheet by atomic and molecular adsorption: First-principles calculations. <i>Chinese Journal of Physics</i> , <b>2019</b> , 57, 1-5	3.5	3
41	Elastic and electronic properties of C2N monolayer: first-principles calculation. <i>Materials Research Express</i> , <b>2019</b> , 6, 025601	1.7	5
40	Hydrogen bond sensing ability of CdSe/ZnS colloidal quantum dots in ionic medium. <i>Materials Research Express</i> , <b>2019</b> , 6, 015016	1.7	
39	Effects of atoms and molecules adsorption on electronic and magnetic properties of s-triazine with embedded Fe atom: DFT investigations. <i>Philosophical Magazine</i> , <b>2018</b> , 98, 1114-1129	1.6	8
38	First-principles studies on the superconductivity of aluminene. <i>Applied Surface Science</i> , <b>2018</b> , 445, 161-1	<b>66</b> 7	18
37	First-principles investigation of graphitic carbon nitride monolayer with embedded Fe atom. <i>Surface Science</i> , <b>2018</b> , 667, 112-120	1.8	18
36	Molecular dynamics simulation of melting of silicene. <i>Materials Research Express</i> , <b>2018</b> , 5, 065054	1.7	7
35	Selective hydrogen adsorption on a buckled carbon nitride sheet: first-principles calculation. <i>Materials Research Express</i> , <b>2018</b> , 5, 125605	1.7	6
34	Functionalization of single-layer Pmma-CO by adatoms: A first-principles study of electronic, magnetic and structural properties. <i>Journal of Physics and Chemistry of Solids</i> , <b>2018</b> , 123, 294-299	3.9	3
33	High-pressure phases of AlxIn1⊠N compounds: First principles calculations. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 704, 160-169	5.7	8

32	Investigation of Melting Dynamics of Hafnium Clusters. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 517-528	6.1	1
31	Theoretical studies on mechanical and electronic properties of s-triazine sheet. <i>Philosophical Magazine</i> , <b>2017</b> , 97, 2077-2088	1.6	11
30	Molecular dynamics simulations and photoluminescence measurements of annealed ZnO surfaces. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2017</b> , 90, 28-36	3	2
29	Thermoelectric and piezoelectric properties of the predicted AllnN composites based on ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 24613-24625	3.6	2
28	First-principles studies on the effects of halogen adsorption on monolayer antimony. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 25786-25795	3.6	11
27	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. <i>Computer Physics Communications</i> , <b>2017</b> , 220, 143-149	4.2	17
26	Effects of Hubbard term correction on the structural parameters and electronic properties of wurtzite ZnO. <i>Computational Materials Science</i> , <b>2017</b> , 138, 111-116	3.2	32
25	Theory of d-Wave High Temperature Superconductivity in the Cuprates Involving Non-linear Lattice Modes. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2017</b> , 30, 3377-3395	1.5	O
24	Effect of chemical interface damping and aggregation size of bare gold nanoparticles in NaCl on the plasmon resonance damping. <i>Optical Materials Express</i> , <b>2017</b> , 7, 955	2.6	11
23	Resonance position and extinction efficiency of a single silica coated gold nanoshell when size effects of core is matter <b>2017</b> ,		2
22	Structural and response properties of all BaTiO3 phases from density functional theory using the projector-augmented-wave methods. <i>Computational Materials Science</i> , <b>2016</b> , 117, 306-314	3.2	6
21	Geometric and electric properties of graphitic carbon nitride sheet with embedded single manganese atom under bi-axial tensile strain. <i>Current Applied Physics</i> , <b>2016</b> , 16, 809-815	2.6	17
20	Thorough investigations of the structural and electronic properties of AlxIn1-xN ternary compound via ab initio computations. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 682, 338-344	5.7	3
19	Ab initio computations of the linear and nonlinear optical properties of stable compounds in AlInN system. <i>Current Applied Physics</i> , <b>2016</b> , 16, 1277-1283	2.6	5
18	Structural relaxation of BaTiO3 slab with tetragonal (100) surface: Ab-initio comparison of different thickness. <i>Current Applied Physics</i> , <b>2016</b> , 16, 1491-1497	2.6	5
17	Mechanical and electronic properties of graphitic carbon nitride sheet: First-principles calculations. <i>Solid State Communications</i> , <b>2016</b> , 248, 144-150	1.6	25
16	Guided basin-hopping search of small boron clusters with density functional theory 2015,		1
15	Molecular dynamics simulation of annealed ZnO surfaces <b>2015</b> ,		1

## LIST OF PUBLICATIONS

14	Growth of bi- and tri-layered graphene on silicon carbide substrate via molecular dynamics simulation <b>2015</b> ,		1
13	AERONET dataBased determination of aerosol types. <i>Atmospheric Pollution Research</i> , <b>2015</b> , 6, 682-695	4.5	20
12	Monsoonal variations in aerosol optical properties and estimation of aerosol optical depth using ground-based meteorological and air quality data in Peninsular Malaysia. <i>Atmospheric Chemistry and Physics</i> , <b>2015</b> , 15, 3755-3771	6.8	12
11	Multiple regression method to determine aerosol optical depth in atmospheric column in Penang, Malaysia. <i>IOP Conference Series: Earth and Environmental Science</i> , <b>2014</b> , 18, 012081	0.3	1
10	Manipulating API and AOD data to distinguish transportation of aerosol at high altitude in Penang, Malaysia. <i>IOP Conference Series: Earth and Environmental Science</i> , <b>2014</b> , 18, 012082	0.3	O
9	Magnetic Moments due to Orbital Currents in an Electron-Lattice Model of Cuprate Superconductors. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2014</b> , 27, 2673-2677	1.5	1
8	A molecular dynamics study of the thermodynamic properties of barium zirconate. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2013</b> , 21, 045001	2	4
7	X-ray diffraction experiments, luminescence measurements and first-principles GGA+U calculations on YTaO4. <i>Computational Materials Science</i> , <b>2013</b> , 77, 13-18	3.2	13
6	Molecular dynamics study of thermal expansion and isothermal compressibility of strontium titanate and barium zirconate <b>2013</b> ,		1
5	Epitaxial growth of graphene on 6H-silicon carbide substrate by simulated annealing method. Journal of Chemical Physics, 2013, 139, 204702	3.9	13
4	Molecular dynamics simulation of thermodynamic and thermal transport properties of strontium titanate with improved potential parameters. <i>Computational Materials Science</i> , <b>2012</b> , 60, 123-129	3.2	15
3	Surface and interface phonon polaritons of wurtzite GaN thin film grown on 6H-SiC substrate. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 241912	3.4	23
2	Solutions of the atmospheric, solar, and LSND neutrino anomalies from TeV scale quark-lepton unification. <i>Physical Review D</i> , <b>2001</b> , 65,	4.9	2
1	Maximal <b>(b</b> scillations, the see-saw mechanism and the Exact Parity Model. <i>Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics,</i> <b>2000</b> , 491, 291-296	4.2	3