Tiem Leong Yoon

List of Publications by Citations

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

#	Paper	IF	Citations
67	Effects of Hubbard term correction on the structural parameters and electronic properties of wurtzite ZnO. *Computational Materials Science*, **2017**, 138, 111-116	3.2	32
66	Mechanical and electronic properties of graphitic carbon nitride sheet: First-principles calculations. *Solid State Communications*, **2016**, 248, 144-150	1.6	25
65	Surface and interface phonon polaritons of wurtzite GaN thin film grown on 6H-SiC substrate. *Applied Physics Letters*, **2009**, 94, 241912	3.4	23
64	AERONET data‐based determination of aerosol types. *Atmospheric Pollution Research*, **2015**, 6, 682-695	4.5	20
63	First-principles studies on the superconductivity of aluminene. *Applied Surface Science*, **2018**, 445, 161-166	6.7	18
62	First-principles investigation of graphitic carbon nitride monolayer with embedded Fe atom. *Surface Science*, **2018**, 667, 112-120	1.8	18
61	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	4.2	17
60	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	2.6	17
59	Molecular dynamics simulation of thermodynamic and thermal transport properties of strontium titanate with improved potential parameters. *Computational Materials Science*, **2012**, 60, 123-129	3.2	15
58	X-ray diffraction experiments, luminescence measurements and first-principles GGA+U calculations on YTaO4. *Computational Materials Science*, **2013**, 77, 13-18	3.2	13
57	Epitaxial growth of graphene on 6H-silicon carbide substrate by simulated annealing method. *Journal of Chemical Physics*, **2013**, 139, 204702	3.9	13
56	First-principles study of monolayer Be2C as an anode material for lithium-ion batteries. *Journal of Applied Physics*, **2019**, 126, 125302	2.5	12
55	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	6.8	12
54	Theoretical studies on mechanical and electronic properties of s-triazine sheet. *Philosophical Magazine*, **2017**, 97, 2077-2088	1.6	11
53	First-principles studies on the effects of halogen adsorption on monolayer antimony. *Physical Chemistry Chemical Physics*, **2017**, 19, 25786-25795	3.6	11
52	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	2.6	11
51	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	5.1	9

50	High-pressure phases of AlxIn1−xN compounds: First principles calculations. *Journal of Alloys and Compounds*, **2017**, 704, 160-169	5.7	8
49	Metal-free ferromagnetic semiconductor: Mechanical, electronic and magnetic properties of boron doped graphitic carbon nitride (g-C6N6) sheet. *Materials Chemistry and Physics*, **2020**, 254, 123470	4.4	8
48	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	1.6	8
47	Strain-tunable electronic and magnetic properties of two-dimensional gallium nitride with vacancy defects. *Journal of Applied Physics*, **2020**, 127, 015305	2.5	8
46	Monolayer GaN functionalized with alkali metal and alkaline earth metal atoms: A first-principles study. *Superlattices and Microstructures*, **2019**, 130, 428-436	2.8	7
45	Molecular dynamics simulation of melting of silicene. *Materials Research Express*, **2018**, 5, 065054	1.7	7
44	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	3.2	6
43	Selective hydrogen adsorption on a buckled carbon nitride sheet: first-principles calculation. *Materials Research Express*, **2018**, 5, 125605	1.7	6
42	Ab initio computations of the linear and nonlinear optical properties of stable compounds in AlInN system. *Current Applied Physics*, **2016**, 16, 1277-1283	2.6	5
41	Structural relaxation of BaTiO3 slab with tetragonal (100) surface: Ab-initio comparison of different thickness. *Current Applied Physics*, **2016**, 16, 1491-1497	2.6	5
40	Frequency dependent linear and nonlinear optical properties of compositionally tuned inorganic CsSnX (X = Br, I) composites. *Journal of Alloys and Compounds*, **2019**, 779, 497-504	5.7	5
39	Elastic and electronic properties of C2N monolayer: first-principles calculation. *Materials Research Express*, **2019**, 6, 025601	1.7	5
38	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	4.8	5
37	Integrated SnSSe bulk and monolayer as industrial waste heat thermoelectric materials. *International Journal of Energy Research*, **2021**, 45, 2085-2099	4.5	5
36	A molecular dynamics study of the thermodynamic properties of barium zirconate. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 045001	2	4
35	An efficient Monte Carlo fission source convergence acceleration strategy adapted from the survival biasing technique. *Annals of Nuclear Energy*, **2020**, 138, 107164	1.7	4
34	Maximal Ɗoscillations, the see-saw mechanism and the Exact Parity Model. *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics*, **2000**, 491, 291-296	4.2	3
33	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	5.7	3

32	Biogas detection on carbon nitride sheet with embedded Mn atom: dispersion-corrected density functional theory. *Materials Research Express*, **2019**, 6, 065603	1.7	3
31	The development of a multigroup Monte Carlo code for TRIGA reactors. *Nuclear Engineering and Design*, **2019**, 342, 99-114	1.8	3
30	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	3.5	3
29	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	3.9	3
28	Molecular dynamics simulations and photoluminescence measurements of annealed ZnO surfaces. *Physica E: Low-Dimensional Systems and Nanostructures*, **2017**, 90, 28-36	3	2
27	Thermoelectric and piezoelectric properties of the predicted AlInN composites based on ab initio calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 24613-24625	3.6	2
26	Solutions of the atmospheric, solar, and LSND neutrino anomalies from TeV scale quark-lepton unification. *Physical Review D*, **2001**, 65,	4.9	2
25	Resonance position and extinction efficiency of a single silica coated gold nanoshell when size effects of core is matter **2017**,		2
24	Investigation of Melting Dynamics of Hafnium Clusters. *Journal of Chemical Information and Modeling*, **2017**, 57, 517-528	6.1	1
23	Multiple regression method to determine aerosol optical depth in atmospheric column in Penang, Malaysia. *IOP Conference Series: Earth and Environmental Science*, **2014**, 18, 012081	0.3	1
22	Guided basin-hopping search of small boron clusters with density functional theory **2015**,		1
21	Molecular dynamics simulation of annealed ZnO surfaces **2015**,		1
20	Growth of bi- and tri-layered graphene on silicon carbide substrate via molecular dynamics simulation **2015**,		1
19	Magnetic Moments due to Orbital Currents in an Electron-Lattice Model of Cuprate Superconductors. *Journal of Superconductivity and Novel Magnetism*, **2014**, 27, 2673-2677	1.5	1
18	Molecular dynamics study of thermal expansion and isothermal compressibility of strontium titanate and barium zirconate **2013**,		1
17	Magnetic resonance imaging (MRI) compatible ZrX (X = Hf, Mo and Ru) alloys with enhanced mechanical properties as alternative biomedical applications. *Scripta Materialia*, **2020**, 178, 82-85	5.6	1
16	Metal to semiconductor transition of two-dimensional NbSe2 through hydrogen adsorption: A first-principles study. *Journal of Applied Physics*, **2020**, 128, 105301	2.5	1
15	Halogenated monolayer SnS: a first-principles studies. *IOP Conference Series: Materials Science and Engineering*, **2019**, 625, 012001	0.4	1

14	DFTB parameterization and its application for the global minimum search of the small boron-carbon clusters. *Chemical Physics Letters*, **2019**, 716, 207-210	2.5	1
13	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. *International Journal of Quantum Chemistry*, **2019**, 119, e25884	2.1	1
12	Effects of oxygen variation on the improved structural stability, electronic and optical properties of ZnTeO compounds. *Journal of Physics Condensed Matter*, **2020**, 32, 225701	1.8	1
11	Electronics and magnetic properties of p-block elements doped 2D buckled gallium nitride MGaN (M = Al, Si, P and S): A first-principles study **2021**,		1
10	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	4.4	1
9	Mechanical and optical properties of polymeric nitrogen achieved by compression: DFT study. *Materialia*, **2021**, 20, 101206	3.2	1
8	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	0.3	0
7	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	1.5	0
6	Adsorption and decomposition of H2S on C2N sheet with embedded manganese atom: First-principles calculations. *Chemical Physics*, **2022**, 555, 111443	2.3	0
5	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	2.4	0
4	A first-principles study of two-dimensional NbSeH/g-ZnO van der Waals heterostructures as a water splitting photocatalyst. *Physical Chemistry Chemical Physics*, **2021**, 23, 24222-24232	3.6	0
3	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. *International Journal of Quantum Chemistry*, **2020**, 120, e26079	2.1	
2	Hydrogen bond sensing ability of CdSe/ZnS colloidal quantum dots in ionic medium. *Materials Research Express*, **2019**, 6, 015016	1.7	
1	New phase of lead chalcogenide alloy: Ternary alloy PbSrSe2 for future thermoelectric application. *Materialia*, **2022**, 23, 101443	3.2	