Nawee Kungwan

List of Publications by Citations

158 papers	2,316 citations	23 h-index	36 g-index
163 ext. papers	2,816 ext. citations	4.2 avg, IF	5.47 L-index

#	Paper	IF	Citations
158	Manipulation of Amorphous-to-Crystalline Transformation: Towards the Construction of Covalent Organic Framework Hybrid Microspheres with NIR Photothermal Conversion Ability. *Angewandte Chemie - International Edition*, **2016**, 55, 13979-13984	16.4	218
157	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2'-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 9016-25	3.6	60
156	Kinetics of the hydrogen abstraction *CH3 + alkane --> CH4 + alkyl reaction class: an application of the reaction class transition state theory. *Journal of Physical Chemistry A*, **2005**, 109, 7742-50	2.8	54
155	Manipulation of Amorphous-to-Crystalline Transformation: Towards the Construction of Covalent Organic Framework Hybrid Microspheres with NIR Photothermal Conversion Ability. *Angewandte Chemie*, **2016**, 128, 14185-14190	3.6	45
154	Stepwise double excited-state proton transfer is not possible in 7-azaindole dimer. *Chemical Science*, **2015**, 6, 5762-5767	9.4	42
153	Binding mode and free energy prediction of fisetin/Ecyclodextrin inclusion complexes. *Beilstein Journal of Organic Chemistry*, **2014**, 10, 2789-99	2.5	42
152	A MnN4 moiety embedded graphene as a magnetic gas sensor for CO detection: A first principle study. *Applied Surface Science*, **2019**, 473, 820-827	6.7	41
151	Complete reaction mechanisms of mercury oxidation on halogenated activated carbon. *Journal of Hazardous Materials*, **2016**, 310, 253-60	12.8	40
150	Theoretical investigation of novel carbazole-fluorene based D-EA conjugated organic dyes as dye-sensitizer in dye-sensitized solar cells (DSCs). *Journal of Computational Chemistry*, **2011**, 32, 1568-76	3.5	40
149	Combustion modeling and kinetic rate calculations for a stoichiometric cyclohexane flame. 1. Major reaction pathways. *Journal of Physical Chemistry A*, **2007**, 111, 4102-15	2.8	40
148	Excited-state intermolecular proton transfer reactions of 7-azaindole(MeOH)(n) (n = 1-3) clusters in the gas phase: on-the-fly dynamics simulation. *Journal of Physical Chemistry A*, **2011**, 115, 14129-36	2.8	39
147	Effects of different proton donor and acceptor groups on excited-state intramolecular proton transfers of amino-type and hydroxy-type hydrogen-bonding molecules: theoretical insights. *New Journal of Chemistry*, **2017**, 41, 8761-8771	3.6	36
146	Physical properties and biological activities of hesperetin and naringenin in complex with methylated Ecyclodextrin. *Beilstein Journal of Organic Chemistry*, **2015**, 11, 2763-73	2.5	35
145	Modulation of Solid-State Aggregation of Square-Planar Pt(II) Based Emitters: Enabling Highly Efficient Deep-Red/Near Infrared Electroluminescence. *Advanced Functional Materials*, **2020**, 30, 2002494	15.6	33
144	Dynamics simulations of photoinduced proton transfer reactions of 2-(2?-hydroxyphenyl)benzoxazole in the gas phase and its hydrated clusters. *Chemical Physics Letters*, **2014**, 609, 147-154	2.5	32
143	A 3D-RISM/RISM study of the oseltamivir binding efficiency with the wild-type and resistance-associated mutant forms of the viral influenza B neuraminidase. *Protein Science*, **2016**, 25, 147-58	6.3	30
142	Inclusion complexation of pinostrobin with various cyclodextrin derivatives. *Journal of Molecular Graphics and Modelling*, **2016**, 63, 91-8	2.8	30

141	Effects of linker, anchoring group and capped carbazole at meso-substituted zinc-porphyrins on conversion efficiency of DSSCs. *Dyes and Pigments*, **2015**, 118, 64-75	4.6	28
140	The effect of conjugated spacer on novel carbazole derivatives for dye-sensitized solar cells: density functional theory/time-dependent density functional theory study. *Journal of Computational Chemistry*, **2012**, 33, 1517-23	3.5	28
139	A DFT study of volatile organic compounds adsorption on transition metal deposited graphene. *Applied Surface Science*, **2017**, 396, 1712-1718	6.7	27
138	The effect of protic solvents on the excited state proton transfer of 3-hydroxyflavone: A TD-DFT static and molecular dynamics study. *Journal of Molecular Liquids*, **2018**, 252, 428-438	6	27
137	Triple bond-modified anthracene sensitizers for dye-sensitized solar cells: a computational study. *RSC Advances*, **2015**, 5, 38130-38140	3.7	25
136	Carbon-doped boron nitride nanosheet as a promising metal-free catalyst for NO reduction: DFT mechanistic study. *Applied Catalysis A: General*, **2018**, 557, 79-88	5.1	24
135	Understanding the role of Ru dopant on selective catalytic reduction of NO with NH3 over Ru-doped CeO2 catalyst. *Chemical Engineering Journal*, **2019**, 369, 124-133	14.7	23
134	A DFT study of arsine adsorption on palladium doped graphene: Effects of palladium cluster size. *Applied Surface Science*, **2016**, 367, 552-558	6.7	23
133	Theoretical Insight into Catalytic Propane Dehydrogenation on Ni(111). *Journal of Physical Chemistry C*, **2018**, 122, 14678-14690	3.8	23
132	Theoretical study on the mechanism and kinetics of ring-opening polymerization of cyclic esters initiated by tin(II) n-butoxide. *Computational and Theoretical Chemistry*, **2014**, 1044, 29-35	2	23
131	Theoretical investigation of the charge-transfer properties in different meso-linked zinc porphyrins for highly efficient dye-sensitized solar cells. *Dalton Transactions*, **2014**, 43, 9166-76	4.3	23
130	A theoretical study on the molecular encapsulation of luteolin and pinocembrin with various derivatized beta-cyclodextrins. *Journal of Molecular Structure*, **2019**, 1180, 480-490	3.4	22
129	Theoretical Insights on Solvent Control of Intramolecular and Intermolecular Proton Transfer of 2-(2'-Hydroxyphenyl)benzimidazole. *Journal of Physical Chemistry A*, **2017**, 121, 5773-5784	2.8	21
128	Role of R292K mutation in influenza H7N9 neuraminidase toward oseltamivir susceptibility: MD and MM/PB(GB)SA study. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 917-926	4.2	21
127	Hydrogen storage performance of platinum supported carbon nanohorns: A DFT study of reaction mechanisms, thermodynamics, and kinetics. *International Journal of Hydrogen Energy*, **2018**, 43, 23336-23345	6.7	21
126	Microporous, Self-Segregated, Graphenal Polymer Nanosheets Prepared by Dehydrogenative Condensation of Aza-PAHs Building Blocks in the Solid State. *Chemistry of Materials*, **2017**, 29, 3971-3979	9.6	20
125	Heteroatom effect on photophysical properties of 2-(2?-hydroxyphenyl)benzimidazole and its derivatives as fluorescent dyes: A TD-DFT study. *Journal of Luminescence*, **2017**, 188, 275-282	3.8	20
124	Influence of hydrogen spillover on Pt-decorated carbon nanocones for enhancing hydrogen storage capacity: A DFT mechanistic study. *Physical Chemistry Chemical Physics*, **2018**, 20, 21194-21203	3.6	20

123	Multi-triphenylamine□unctionalized dithienylbenzothiadiazoles as hole-transporting non-doped red emitters for efficient simple solution processed pure red organic light-emitting diodes. *Organic Electronics*, **2015**, 21, 117-125	3.5	19
122	Coumarin-based donor□cceptor organic dyes for a dye-sensitized solar cell: photophysical properties and electron injection mechanism. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	19
121	The complete reaction mechanism of H2S desulfurization on an anatase TiO2 (001) surface: a density functional theory investigation. *Catalysis Science and Technology*, **2017**, 7, 356-365	5.5	19
120	Efficient bifunctional materials based on pyrene- and triphenylamine-functionalized dendrimers for electroluminescent devices. *RSC Advances*, **2015**, 5, 73481-73489	3.7	18
119	Capability of defective graphene-supported Pd13 and Ag13 particles for mercury adsorption. *Applied Surface Science*, **2016**, 364, 166-175	6.7	18
118	Modulation of □spacer of carbazole-carbazole based organic dyes toward high efficient dye-sensitized solar cells. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2017**, 174, 7-16	4.4	18
117	Theoretical investigation on the mechanism and kinetics of the ring-opening polymerization of □caprolactone initiated by tin(II) alkoxides. *Journal of Molecular Modeling*, **2013**, 19, 5377-85	2	18
116	Molecular recognition of naphthoquinone-containing compounds against human DNA topoisomerase II□ATPase domain: A molecular modeling study. *Journal of Molecular Liquids*, **2017**, 247, 374-385	6	17
115	Low susceptibility of asunaprevir towards R155K and D168A point mutations in HCV NS3/4A protease: A molecular dynamics simulation. *Journal of Molecular Graphics and Modelling*, **2019**, 89, 122-130	2.8	17
114	N-Type Superconductivity in an Organic Mott Insulator Induced by Light-Driven Electron-Doping. *Advanced Materials*, **2017**, 29, 1606833	24	17
113	Significant enhancement in the performance of porphyrin for dye-sensitized solar cells: aggregation control using chenodeoxycholic acid. *New Journal of Chemistry*, **2017**, 41, 7081-7091	3.6	16
112	Metadynamics supports molecular dynamics simulation-based binding affinities of eucalyptol and beta-cyclodextrin inclusion complexes. *RSC Advances*, **2017**, 7, 50899-50911	3.7	16
111	Role of Sn promoter in Ni/Al2O3 catalyst for the deoxygenation of stearic acid and coke formation: experimental and theoretical studies. *Catalysis Science and Technology*, **2019**, 9, 3361-3372	5.5	16
110	Electronic and photophysical properties of 2-(2?-hydroxyphenyl)benzoxazole and its derivatives enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect. *Journal of Luminescence*, **2015**, 167, 132-139	3.8	16
109	Atomistic mechanisms underlying the activation of the G protein-coupled sweet receptor heterodimer by sugar alcohol recognition. *Scientific Reports*, **2019**, 9, 10205	4.9	16
108	Push-Pull N-Annulated Perylene-Based Sensitizers for Dye-Sensitized Solar Cells: Theoretical Property Tuning by DFT/TDDFT. *ChemistrySelect*, **2017**, 2, 9829-9837	1.8	15
107	Density functional theory study of elemental mercury adsorption on boron doped graphene surface decorated by transition metals. *Applied Surface Science*, **2016**, 362, 140-145	6.7	15
106	Combined experimental and theoretical investigation on Fluorescence Resonance Energy Transfer of dye loaded on LTL zeolite. *Microporous and Mesoporous Materials*, **2017**, 241, 372-382	5.3	14

105	Modification of D-A-□A configuration toward a high-performance triphenylamine-based sensitizer for dye-sensitized solar cells: a theoretical investigation. *ChemPhysChem*, **2014**, 15, 3809-18	3.2	14
104	Dynamics simulations of excited-state triple proton transfer in 7-azaindole complexes with water, water□methanol and methanol. *Journal of Photochemistry and Photobiology A: Chemistry*, **2013**, 266, 28-36	4.7	14
103	Molecular Dynamics Simulation Reveals the Selective Binding of Human Leukocyte Antigen Alleles Associated with Behçet's Disease. *PLoS ONE*, **2015**, 10, e0135575	3.7	14
102	Molecular insights into inclusion complexes of mansonone E and H enantiomers with various □cyclodextrins. *Journal of Molecular Graphics and Modelling*, **2018**, 79, 72-80	2.8	14
101	Theoretical study on influence of geometry controlling over the excited-state intramolecular proton transfer of 10-hydroxybenzo[h]quinoline and its derivatives. *Computational and Theoretical Chemistry*, **2017**, 1113, 42-51	2	13
100	Effect of surface modification of poly(l-lactide-co-□caprolactone) membranes by low-pressure plasma on support cell biocompatibility. *Surface and Coatings Technology*, **2016**, 306, 328-335	4.4	13
99	How strong is the edge effect in the adsorption of anticancer drugs on a graphene cluster?. *Journal of Molecular Modeling*, **2016**, 22, 85	2	13
98	Theoretical and Experimental Studies on Inclusion Complexes of Pinostrobin and □Cyclodextrins. *Scientia Pharmaceutica*, **2018**, 86,	4.3	13
97	A DFT study of the unusual substrate-assisted mechanism of Serratia marcescens chitinase B reveals the role of solvent and mutational effect on catalysis. *Journal of Molecular Graphics and Modelling*, **2015**, 56, 53-9	2.8	13
96	Computational screening of fatty acid synthase inhibitors against thioesterase domain. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 4114-4125	3.6	13
95	Mechanistic study of CO oxidation by N 2 O over Ag 7 Au 6 cluster investigated by DFT methods. *Applied Catalysis A: General*, **2017**, 538, 99-106	5.1	12
94	Heteroatom substitution effect on electronic structures, photophysical properties, and excited-state intramolecular proton transfer processes of 3-hydroxyflavone and its analogues: A TD-DFT study. *Journal of Molecular Structure*, **2019**, 1195, 280-292	3.4	12
93	Excited-state intramolecular proton transfer reactions of 2,5-bis(2?-benzoxazolyl)hydroquinone and its water cluster exhibiting single and double proton transfer: A TD-DFT dynamics simulation. *Journal of Molecular Liquids*, **2019**, 286, 110889	6	12
92	Excited-state proton-transfer reactions of 7-azaindole with water, ammonia and mixed water□ammonia: microsolvated dynamics simulation. *Molecular Simulation*, **2015**, 41, 1177-1186	2	12
91	Effects of alkoxide alteration on the ring-opening polymerization of □caprolactone initiated by n-Bu3SnOR: a DFT study. *Structural Chemistry*, **2015**, 26, 695-703	1.8	12
90	Metal cluster-deposited graphene as an adsorptive material for m-xylene. *New Journal of Chemistry* , **2015**, 39, 9650-9658	3.6	12
89	Tin (IV) alkoxide initiator design for poly (d-lactide) synthesis using DFT calculations. *Computational and Theoretical Chemistry*, **2013**, 1020, 121-126	2	12
88	Structural dynamics and binding free energy of neral-cyclodextrins inclusion complexes: molecular dynamics simulation. *Molecular Simulation*, **2017**, 43, 1356-1363	2	12

87	Anchoring number-performance relationship of zinc-porphyrin sensitizers for dye-sensitized solar cells: A combined experimental and theoretical study. *Dyes and Pigments*, **2017**, 136, 697-706	4.6	12
86	Binding specificity of polypeptide substrates in NS2B/NS3pro serine protease of dengue virus type 2: A molecular dynamics Study. *Journal of Molecular Graphics and Modelling*, **2015**, 60, 24-33	2.8	12
85	Protein-protein interactions between SWCNT/chitosan/EGF and EGF receptor: a model of drug delivery system. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 1919-29	3.6	11
84	Conformation study of e-cyclodextrin: Replica exchange molecular dynamics simulations. *Carbohydrate Polymers*, **2016**, 141, 99-105	10.3	11
83	Mechanistic study of NO oxidation on Cr phthalocyanine: theoretical insight. *RSC Advances*, **2017**, 7, 8858-8865	3.7	11
82	Theoretical study of linker-type effect in carbazole arbazole-based dyes on performances of dye-sensitized solar cells. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	11
81	Theoretical study on excited-state intermolecular proton transfer reactions of 1H-pyrrolo[3,2-h]quinoline with water and methanol. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	11
80	Effect of tributyltin alkoxides chain length on the ring-opening polymerization of ?-caprolactone: Kinetics studies by non-isothermal DSC. *Thermochimica Acta*, **2015**, 599, 1-7	2.9	10
79	Effect of number and different types of proton donors on excited-state intramolecular single and double proton transfer in bipyridine derivatives: theoretical insights. *New Journal of Chemistry*, **2020**, 44, 8018-8031	3.6	10
78	Effects of the second hydration shell on excited-state multiple proton transfer: dynamics simulations of 7-azaindole:(H2O)15 clusters in the gas phase. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	10
77	Reaction and free-energy pathways of hydrogen activation on partially promoted metal edge of CoMoS and NiMoS: A DFT and thermodynamics study. *Fuel Processing Technology*, **2017**, 166, 217-227	7.2	10
76	Effect of nitrogen substitution and conjugation on photophysical properties and excited state intramolecular proton transfer reactions of methyl salicylate derivatives: Theoretical investigation. *Journal of Photochemistry and Photobiology A: Chemistry*, **2020**, 389, 112267	4.7	10
75	The number density effect of N-substituted dyes on the TiO2 surface in dye sensitized solar cells: a theoretical study. *RSC Advances*, **2015**, 5, 11549-11557	3.7	9
74	Kinetics and thermodynamics analysis for ring-opening polymerization of caprolactone initiated by tributyltin n-butoxide using differential scanning calorimetry. *Journal of Thermal Analysis and Calorimetry*, **2015**, 119, 567-579	4.1	9
73	Revealing the effect of N-content in Fe doped graphene on its catalytic performance for direct oxidation of methane to methanol. *Applied Surface Science*, **2020**, 527, 146833	6.7	9
72	A Cr-phthalocyanine monolayer as a potential catalyst for NO reduction investigated by DFT calculations. *RSC Advances*, **2016**, 6, 20500-20506	3.7	9
71	Theoretical design of coumarin derivatives incorporating auxiliary acceptor with D- A- A configuration for dye-sensitized solar cells. *Journal of Photochemistry and Photobiology A: Chemistry*, **2016**, 322-323, 16-26	4.7	9
70	Combined experimental and theoretical investigation on photophysical properties of trans-azobenzene confined in LTL zeolite: Effect of cis-isomer forming. *Microporous and Mesoporous Materials*, **2014**, 197, 348-357	5.3	9

69	Theoretical Investigation on the Electronic and Optical Properties of Poly(fluorenevinylene) Derivatives as Light-Emitting Materials. *International Journal of Photoenergy*, **2011**, 2011, 1-9	2.1	9
68	Physical Insight on Mechanism of Photoinduced Charge Transfer in Multipolar Photoactive Molecules. *Scientific Reports*, **2018**, 8, 10089	4.9	9
67	Screening of hepatitis C NS5B polymerase inhibitors containing benzothiadiazine core: a steered molecular dynamics. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 1743-1757	3.6	8
66	Formation of Excimers in Isoquinolinyl Pyrazolate Pt(II) Complexes: Role of Cooperativity Effects. *Inorganic Chemistry*, **2020**, 59, 18253-18263	5.1	8
65	A Disposable and Flexible Graphene Electrode Fabricated by Inkjet Printing of an Aqueous Surfactant-free Graphene Oxide Dispersion. *Chemistry Letters*, **2015**, 44, 800-802	1.7	8
64	Influence of butyl group of tin chloride initiators on the non-isothermal DSC ring-opening polymerization of ε-caprolactone: The studies of kinetics, mechanism and polymer synthesis. *Thermochimica Acta*, **2020**, 683, 178458	2.9	8
63	Theoretical investigation of 2-(iminomethyl)phenol in the gas phase as a prototype of ultrafast excited-state intramolecular proton transfer. *Chemical Physics Letters*, **2016**, 657, 113-118	2.5	8
62	Theoretical insights into photoinduced proton transfer of 7-hydroxyquinoline via intermolecular hydrogen-bonded wire of mixed methanol and water. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	8
61	Effects of π-expansion, an additional hydroxyl group, and substitution on the excited state single and double proton transfer of 2-hydroxybenzaldehyde and its relative compounds: TD-DFT static and dynamic study. *New Journal of Chemistry*, **2019**, 43, 19107-19119	3.6	8
60	Binding pattern and susceptibility of epigallocatechin gallate against envelope protein homodimer of Zika virus: A molecular dynamics study. *Journal of Molecular Liquids*, **2019**, 274, 140-147	6	8
59	A Solid-State Luminescent Cd(II) Supramolecular Coordination Framework Based on Mixed Luminophores as a Sensor for Discriminatively Selective Detection of Amine Vapors. *Inorganic Chemistry*, **2020**, 59, 6176-6186	5.1	8
58	Intramolecular hydrogen bond π-enhanced electroluminescence performance of hybridized local and charge transfer (HLCT) excited-state blue-emissive materials. *Journal of Materials Chemistry C*, **2021**, 9, 497-507	7.1	8
57	TD-DFT Study of Absorption and Emission Spectra of 2-(2'-Aminophenyl)benzothiazole Derivatives in Water. *Journal of Fluorescence*, **2017**, 27, 745-754	2.4	7
56	Cavity Closure of 2-Hydroxypropyl-β-Cyclodextrin: Replica Exchange Molecular Dynamics Simulations. *Polymers*, **2019**, 11,	4.5	7
55	Theoretical mechanistic study of CO catalytic oxidation by O2 on an ultra-small 13-atom bimetallic Ag7Au6 cluster. *Applied Catalysis A: General*, **2020**, 595, 117505	5.1	7
54	Local structure elucidation and reaction mechanism of light naphtha aromatization over Ga embedded H-ZSM-5 zeolite: Combined DFT and experimental study. *Microporous and Mesoporous Materials*, **2020**, 306, 110414	5.3	7
53	Kinetic and mechanistic investigation of the ring-opening polymerization of l-lactide initiated by nBu3SnOnBu using 1H-NMR. *Reaction Kinetics, Mechanisms and Catalysis*, **2016**, 119, 381-392	1.6	7
52	Application of the reaction class transition state theory to the kinetics of hydrogen abstraction reactions of alkanes by atomic chlorine. *Computational and Theoretical Chemistry*, **2013**, 1011, 65-74	2	7

51	Electrochemical Detection of Human Interleukin-15 using a Graphene Oxide-Modified Screen-Printed Carbon Electrode. *Analytical Letters*, **2017**, 50, 1112-1125	2.2	7
50	Theoretical Insights into Excited-State Intermolecular Proton Transfers of 2,7-Diazaindole in Water Using a Microsolvation Approach. *Journal of Physical Chemistry A*, **2021**, 125, 5314-5325	2.8	7
49	Computational screening of chalcones acting against topoisomerase II and their cytotoxicity towards cancer cell lines. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 134-143	5.6	7
48	Comparison of Implicit and Explicit Solvation Models for Iota-Cyclodextrin Conformation Analysis from Replica Exchange Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2017**, 57, 778-786	6.1	6
47	Influence of phenyl-attached substituents on the vibrational and electronic spectra of meso-tetraphenylporphyrin: A DFT study. *Computational and Theoretical Chemistry*, **2015**, 1062, 1-10	2	6
46	Theoretical study of efficiency comparison of Ti (IV) alkoxides as initiators for ring-opening polymerization of caprolactone. *Computational and Theoretical Chemistry*, **2016**, 1090, 17-22	2	6
45	Glycan binding and specificity of viral influenza neuraminidases by classical molecular dynamics and replica exchange molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 3354-3365	3.6	6
44	Organic sensitizers with modified di(thiophen-2-yl)phenylamine donor units for dye-sensitized solar cells: a computational study. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	6
43	A TD-DFT molecular screening for fluorescence probe based on excited-state intramolecular proton transfer of 2hydroxychalcone derivatives. *Journal of Photochemistry and Photobiology A: Chemistry*, **2021**, 410, 113165	4.7	6
42	Oxotitanium-porphyrin for selective catalytic reduction of NO by NH3: a theoretical mechanism study. *New Journal of Chemistry*, **2018**, 42, 16806-16813	3.6	6
41	Imidazole-based solid-state fluorophores with combined ESIPT and AIE features as self-absorption-free non-doped emitters for electroluminescent devices. *Dyes and Pigments*, **2021**, 193, 109488	4.6	6
40	Interactions of HLA-DR and Topoisomerase I Epitope Modulated Genetic Risk for Systemic Sclerosis. *Scientific Reports*, **2019**, 9, 745	4.9	5
39	Encapsulation of alpha-mangostin and hydrophilic beta-cyclodextrins revealed by all-atom molecular dynamics simulations. *Journal of Molecular Liquids*, **2019**, 288, 110965	6	5
38	Catalytic reduction mechanism of deoxygenation of NO via the CO-reaction pathway using nanoalloy Ag7Au6 clusters: density functional theory investigation. *New Journal of Chemistry*, **2018**, 42, 14120-14127	3.6	5
37	DSC Kinetics Analysis for the Synthesis of Three-Arms Poly(caprolactone) Using Aluminum Tri-sec-Butoxide as Initiator. *International Journal of Chemical Kinetics*, **2015**, 47, 734-743	1.4	5
36	Theoretical Study on Factors Influencing the Efficiency of D?A?A Isoindigo-Based Sensitizer for Dye-Sensitized Solar Cells. *Journal of Electronic Materials*, **2020**, 49, 318-332	1.9	5
35	Effect of D168V mutation in NS3/4A HCV protease on susceptibilities of faldaprevir and danoprevir. *Molecular BioSystems*, **2016**, 12, 3666-3673		5
34	Theoretical Prediction and Analysis of the UV/Visible Absorption and Emission Spectra of Chiral Carbon Nanorings. *Journal of Physical Chemistry A*, **2018**, 122, 7284-7292	2.8	5

33	Theoretical analysis of orientations and tautomerization of genistein in Cyclodextrin. *Journal of Molecular Liquids*, **2018**, 265, 16-23	6	5
32	Theoretical study of heteroatom and substituent effects on excited-state intramolecular proton transfers and electronic properties of amino-type hydrogen bonding molecules. *Journal of Luminescence*, **2021**, 238, 118260	3.8	5
31	Theoretical guidance and experimental confirmation on catalytic tendency of M-CeO2 (M = Zr, Mn, Ru or Cu) for NH3-SCR of NO. *Molecular Simulation*, **2017**, 43, 1240-1246	2	4
30	Location and reactivity of extra-framework cation in the alkali exchanged LTL zeolites: A periodic density functional study. *Microporous and Mesoporous Materials*, **2014**, 195, 227-239	5.3	4
29	LC-BLYP Calculations of the Structures and Photophysical Properties of [1,3]Thiazolo[4,5-]pyrazine Derivatives in Cyclohexane and Methanol. *Journal of Physical Chemistry A*, **2019**, 123, 10685-10693	2.8	4
28	Effect of Water Microsolvation on the Excited-State Proton Transfer of 3-Hydroxyflavone Enclosed in Cyclodextrin. *Molecules*, **2021**, 26,	4.8	4
27	The inclusion complexation of daidzein with cyclodextrin and 2,6-dimethyl-cyclodextrin: a theoretical and experimental study. *Monatshefte F Chemie*, **2018**, 149, 1739-1747	1.4	4
26	Tunable keto emission of 2-(2?-hydroxyphenyl)benzothiazole derivatives with expansion, substitution and additional proton transfer site for excited-state proton transfer-based fluorescent probes: Theoretical insights. *Journal of Photochemistry and Photobiology A: Chemistry*, **2021**, 419, 113450	4.7	4
25	Nuclear quantum effect and temperature dependency on the hydrogen-bonded structure of 7-azaindole dimer. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	3
24	Synthesis, physical and electroluminescence properties of 3,6-dipyrenylcarbazole end capped oligofluorenes. *RSC Advances*, **2015**, 5, 26569-26579	3.7	3
23	Electroanalytical Application of Screen-printed Carbon Electrode Modified with Conductive Graphene OxidePoly(acrylic acid) Film for Label-free Detection of Human Immunoglobulin G. *Chemistry Letters*, **2016**, 45, 1444-1446	1.7	3
22	Susceptibility of inhibitors against 3C protease of coxsackievirus A16 and enterovirus A71 causing hand, foot and mouth disease: A molecular dynamics study. *Biophysical Chemistry*, **2016**, 219, 9-16	3.5	3
21	Asymmetric hydrogen bonding in formic acidnitric acid dimer observed by quantum molecular dynamics simulations. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	2
20	Theoretical rationalization for reduced charge recombination in bulky carbazole-based sensitizers in solar cells. *Journal of Computational Chemistry*, **2017**, 38, 901-909	3.5	2
19	Influence of Molecular Weight on the Non-Isothermal Melt Crystallization of Biodegradable Poly(D-Lactide). *Key Engineering Materials*, **2017**, 751, 221-229	0.4	2
18	The Role of Metal Species on Aldehyde Hydrogenation over Co13 and Ni13 Supported on Al2O3(110) Surfaces: A Theoretical Study. *ChemistrySelect*, **2020**, 5, 4058-4068	1.8	2
17	Structure and electronic properties of deformed single-walled carbon nanotubes: quantum calculations. *Structural Chemistry*, **2018**, 29, 39-47	1.8	2
16	Rapid activity prediction of HIV-1 integrase inhibitors: harnessing docking energetic components for empirical scoring by chemometric and artificial neural network approaches. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 471-88	4.2	2

15	A spectroscopic study of indigo dye in aqueous solution: A combined experimental and TD-DFT study. *Journal of Luminescence*, **2018**, 204, 568-572	3.8	2
14	Solvent Dependence of Double Proton Transfer in the Formic Acid-Formamidine Complex: Path Integral Molecular Dynamics Investigation. *Journal of Physical Chemistry A*, **2017**, 121, 7324-7334	2.8	2
13	Synthesis, Thermal, Optical and Electrochemical Properties of Acridone and Thioxanthone Based Push-Pull Molecules. *ChemistrySelect*, **2020**, 5, 15180-15189	1.8	2
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