

Kittusamy Senthilkumar

List of Publications by Year in descending order

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123
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3372
citing authors

#	ARTICLE	IF	CITATIONS
1	Charge Transport Properties in Discotic Liquid Crystals: A Quantum-Chemical Insight into Structure-Property Relationships. <i>Journal of the American Chemical Society</i> , 2004, 126, 3271-3279.	13.7	464
2	Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies. <i>Journal of Chemical Physics</i> , 2003, 119, 9809-9817.	3.0	395
3	Absolute Rates of Hole Transfer in DNA. <i>Journal of the American Chemical Society</i> , 2005, 127, 14894-14903.	13.7	325
4	Mapping the Sites for Selective Oxidation of Guanines in DNA. <i>Journal of the American Chemical Society</i> , 2003, 125, 13658-13659.	13.7	97
5	N-heterocycles as corrosion inhibitors for mild steel in acid medium. <i>Journal of Molecular Liquids</i> , 2016, 216, 42-52.	4.9	94
6	Charge Transport in Self-Organized π -Stacks of p-Phenylene Vinylene Oligomers. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18267-18274.	2.6	90
7	Graphene Quantum Dot Solid Sheets: Strong blue-light-emitting & photocurrent-producing band-gap-opened nanostructures. <i>Scientific Reports</i> , 2017, 7, 10850.	3.3	61
8	Calculation of ionization potential and chemical hardness: A comparative study of different methods. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 764-771.	2.0	59
9	Copper(I) hydrazone complexes: Synthesis, structure, DNA binding, radical scavenging and computational studies. <i>Inorganic Chemistry Communication</i> , 2011, 14, 1318-1322.	3.9	53
10	Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds. <i>Journal of the Royal Society Interface</i> , 2008, 5, 207-216.	3.4	49
11	Quantum chemical studies on tautomerism of barbituric acid in gas phase and in solution. <i>Journal of Computer-Aided Molecular Design</i> , 2002, 16, 263-272.	2.9	47
12	Optical Absorption and Emission Properties of Fluoranthene, Benzo[k]fluoranthene, and Their Derivatives. A DFT Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14647-14656.	2.5	41
13	Ultrasonic, DFT and FT-IR studies on hydrogen bonding interactions in aqueous solutions of diethylene glycol. <i>Journal of Molecular Liquids</i> , 2015, 202, 115-124.	4.9	38
14	Structural and Spectral Properties of 4-Bromo-1-naphthyl Chalcones: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6594-6602.	2.5	36
15	Ab initio and DFT studies on structure and stability of aliphatic aldoxime molecules. <i>Computational and Theoretical Chemistry</i> , 2001, 535, 61-70.	1.5	33
16	Coordination Behavior of Acylthiourea Ligands in Their Ru(II) Benzene Complexes Structures and Anticancer Activity. <i>Organometallics</i> , 2022, 41, 1621-1630.	2.3	33
17	Effect of structural fluctuations on charge carrier mobility in thiophene, thiazole and thiazolothiazole based oligomers. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17947.	2.8	32
18	Theoretical and experimental evaluation of a new organic proton transfer crystal aminoguanidinium p-nitrobenzoate monohydrate for optical limiting applications. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 111, 82-94.	4.0	31

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19	Theoretical studies on the quinoidal thiophene based dyes for dye sensitized solar cell and NLO applications. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21496-21505.	2.8	30
20	Copper Ion Mediated Selective Cleavage of C-S Bond in Ferrocenylthiosemicarbazone Forming Mixed Geometrical [(PPh ₃) ₃ Cu(1/4-S) ₂ Cu(PPh ₃) ₃] ₂ Having Cu ₂ S ₂ Core: Toward a New Avenue in Copper-Sulfur Chemistry. <i>Inorganic Chemistry</i> , 2012, 51, 3525-3532.	4.0	29
21	Graphene Nanobuds: A New Second-Generation Phosgene Sensor with Ultralow Detection Limit in Aqueous Solution. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 19339-19349.	8.0	27
22	Interactions of anticancer drugs with usual and mismatch base pairs - Density functional theory studies. <i>Biophysical Chemistry</i> , 2008, 136, 50-58.	2.8	26
23	Mechanism and Kinetics of the Atmospheric Oxidative Degradation of Dimethylphenol Isomers Initiated by OH Radical. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4611-4626.	2.5	26
24	Synthesis and characterization studies of ZnSe quantum dots. <i>Journal of Materials Science: Materials in Electronics</i> , 2012, 23, 2048-2052.	2.2	25
25	Theoretical studies on the reaction mechanism and kinetics of the atmospheric reactions of 1,4-thioxane with OH radical. <i>Structural Chemistry</i> , 2012, 23, 1475-1488.	2.0	25
26	Theoretical investigation of interaction between psoralen and altretamine with stacked DNA base pairs. <i>Materials Science and Engineering C</i> , 2012, 32, 423-431.	7.3	25
27	Theoretical investigation on the structure and antioxidant activity of (+) catechin and (-) epicatechin - a comparative study. <i>Molecular Physics</i> , 2020, 118, e1745917.	1.7	24
28	Two-Dimensional Charge Delocalization in X-Shaped Phenylenevinylene Oligomers. <i>Chemistry of Materials</i> , 2006, 18, 2118-2129.	6.7	23
29	Oxidation and Nitration of Tyrosine by Ozone and Nitrogen Dioxide: Reaction Mechanisms and Biological and Atmospheric Implications. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3479-3490.	2.6	23
30	Structural diversity in aroylthiourea copper complexes - formation and biological evaluation of [Cu(<i>trans</i> -SCl)] ₂ , <i>cis</i> -Cu(<i>trans</i>) ₂ O ₂ , <i>trans</i> -Cu(<i>trans</i>) ₂ O ₂ and Cu(<i>trans</i>) ₃ cores. <i>New Journal of Chemistry</i> , 2016, 40, 5401-5413.	2.8	23
31	Wurtzite ZnSe quantum dots: synthesis, characterization and PL properties. <i>Journal of Materials Science: Materials in Electronics</i> , 2013, 24, 692-696.	2.2	22
32	Post Hartree-Fock and density functional theory studies on structure and conformational stability of nitrosoethylene and substituted compounds of nitrosoethylene. <i>Computers & Chemistry</i> , 2002, 26, 207-221.	1.2	20
33	The atmospheric oxidation mechanism and kinetics of 1,3,5-trimethylbenzene initiated by OH radicals - a theoretical study. <i>New Journal of Chemistry</i> , 2017, 41, 10259-10271.	2.8	19
34	Origin of the cis effect - nonbonded intramolecular interactions: quantum chemical studies on 1,2-dihaloethylene molecules. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 95-102.	1.5	18
35	Tautomerization and solvent effects on the absorption and emission properties of the Schiff base <i>N,N'</i> -bis(salicylidene)- <i>p</i> -phenylenediamine - A TDDFT study. <i>Molecular Physics</i> , 2010, 108, 1817-1827.	1.7	18
36	Structural, optical, and charge transport properties of cyclopentadithiophene derivatives: a theoretical study. <i>Structural Chemistry</i> , 2014, 25, 715-731.	2.0	18

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37	Absorption and emission properties of phenylene ethynylene oligomers: effect of substitution and π -conjugation length. <i>Molecular Physics</i> , 2009, 107, 1629-1639.	1.7	17
38	Lennard-Jones Parameters for B3LYP/CHARMM27 QM/MM Modeling of Nucleic Acid Bases. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 396-410.	5.3	17
39	Structure and spectral properties of l-histidinium dipicrate dihydrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 102-111.	3.9	17
40	Triazolyl-donor-acceptor chromophore-decorated unnatural amino acids and peptides: FRET events in a β -turn conformation. <i>Chemical Communications</i> , 2014, 50, 433-435.	4.1	17
41	Adsorption of RGD tripeptide on anatase (001) surface – A first principle study. <i>Computational Materials Science</i> , 2015, 104, 124-129.	3.0	16
42	Ab Initio QM/MM Modeling of the Rate-Limiting Proton Transfer Step in the Deamination of Tryptamine by Aromatic Amine Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9785-9798.	2.6	16
43	Charge Transfer in Polypeptides: Effect of Secondary Structures on Charge-Transfer Integral and Site Energies. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11551-11556.	2.5	15
44	Charge transport and optical properties of cross-conjugated organic molecules: A theoretical study. <i>Organic Electronics</i> , 2014, 15, 1607-1623.	2.6	15
45	Effect of Structural Fluctuations on Charge Carrier Dynamics in Triazene Based Octupolar Molecules. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27754-27762.	3.1	14
46	A theoretical study on optical and charge transport properties of anthra-[1,2-b:4,3-b':5,6-b''':8,7-b''']tetrathiophene molecules. <i>Chemical Physics</i> , 2014, 433, 48-59.	1.9	14
47	Mechanism and Kinetics of the Reaction of Nitrosamines with OH Radical: A Theoretical Study. <i>International Journal of Chemical Kinetics</i> , 2017, 49, 339-353.	1.6	14
48	Mechanism and kinetics of diuron oxidation by hydroxyl radical addition reaction. <i>Environmental Science and Pollution Research</i> , 2020, 27, 12080-12095.	5.3	14
49	Structure, conformation and NMR studies on 1,2-dioxane and halogen substituted 1,2-dioxane molecules. <i>Computational Biology and Chemistry</i> , 2003, 27, 173-183.	2.3	13
50	Structural properties and the effect of platinum drugs with DNA base pairs. <i>Structural Chemistry</i> , 2013, 24, 583-595.	2.0	13
51	Dissociation of N ₂ O on anatase TiO ₂ (001) surface – The effect of oxygen vacancy and presence of Ag cluster. <i>Applied Surface Science</i> , 2016, 389, 1220-1232.	6.1	13
52	Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical: Hydrogen and Chlorine Atom Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8954-8967.	2.5	13
53	Investigation on surface interaction between graphene nanobuds and cerium(III) via fluorescence excimer, theoretical, real water sample, and bioimaging studies. <i>Materials Chemistry and Physics</i> , 2021, 264, 124453.	4.0	13
54	Hartree-Fock and density functional theory studies on ionization and fragmentation of halomethane molecules by positron impact. <i>Molecular Physics</i> , 2002, 100, 3817-3822.	1.7	12

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55	Effect of substitution of electron-donating and -withdrawing groups on the stability of flavin- π -diaminepyridine complexes—a density functional theory study. Computational and Theoretical Chemistry, 2006, 758, 107-112.	1.5	12
56	Reaction mechanism of cysteine proteases model compound HSH with diketone inhibitor PhCOCOCH ₃ X _n , (X = F, Cl, n = 0, 1, 2). International Journal of Quantum Chemistry, 2010, 110, 1660-1674.	2.0	12
57	Atmospheric Oxidation Mechanism and Kinetics of Hydrofluoroethers, CH ₃ OCF ₃ , CH ₃ OCHF ₂ , and CHF ₂ OCH ₂ CF ₃ , by OH Radical: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 4972-4982.	2.5	12
58	Structural properties and the effect of interaction of alkali (Li ⁺ , Na ⁺ , K ⁺) and alkaline earth (Be ²⁺ , Mg ²⁺) on the structural properties of the Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 57-65.	2.5	11
59	Understanding the absorption and emission spectra of borondipyrromethene dye and its substituted analogues. Molecular Physics, 2012, 110, 445-456.	1.7	11
60	Aggregation induced emission behavior in oleylamine acetone system and its application to get improved photocurrent from In ₂ S ₃ quantum dots. Scientific Reports, 2020, 10, 19712.	3.3	11
61	Insight into the photophysics of strong dual emission (blue & green) producing graphene quantum dot clusters and their application towards selective and sensitive detection of trace level Fe ³⁺ and Cr ⁶⁺ ions. RSC Advances, 2020, 10, 26613-26630.	3.6	11
62	Hydrogen-bonding studies of amino acid side-chains with DNA base pairs. Molecular Physics, 2011, 109, 1995-2008.	1.7	10
63	Hydrogen bond interactions in hydrated acetylsalicylic acid. Computational and Theoretical Chemistry, 2011, 966, 167-179.	2.5	10
64	A theoretical study of structural and electronic properties of pentacene/Al(1 0 0) interface. Journal of Molecular Graphics and Modelling, 2012, 38, 334-341.	2.4	10
65	Effect of dynamic disorder on charge carrier dynamics in Ph4DP and Ph4DTP molecules. RSC Advances, 2015, 5, 38722-38732.	3.6	10
66	Opto-electronic and interfacial charge transfer properties of azobenzene dyes on anatase TiO ₂ (001) surface—the effect of anchoring group. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 346, 372-381.	3.9	10
67	A theoretical investigation on the mechanism and kinetics of the gas-phase reaction of naphthalene with OH radical. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	9
68	Effect of site energy fluctuation on charge transport in disordered organic molecules. Journal of Chemical Physics, 2019, 151, 224301.	3.0	9
69	Structural properties and the effect of 2,6-diaminoanthraquinone on π -tetrads, non- π -tetrads, and mixed tetrads—a density functional theory study. International Journal of Quantum Chemistry, 2011, 111, 3239-3250.	2.0	8
70	First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes—a Ab initio and DFT study. Polyhedron, 2011, 30, 1431-1445.	2.2	8
71	Mechanism and kinetics of the reaction of 1,4-thioxane with O ₃ in the atmosphere—a theoretical study. Chemical Physics Letters, 2012, 525-526, 153-159.	2.6	8
72	Theoretical and experimental studies on the structure and spectroscopic properties of Ni(II) complexes of the type [Ni(L)(PPh ₃)] [H ₂ L=5-methyl-N-(2-mercaptophenyl)salicylideneimine and 5-chloro-N-(2-mercaptophenyl)salicylideneimine]. Journal of Molecular Structure, 2013, 1037, 367-375.	3.6	8

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73	Simultaneous Reduction of NO _x and Soot Using Early Post Injection. , 0, , .		8
74	Theoretical studies on charge transport and optical properties of tris(N-saclicylideneanilines). RSC Advances, 2014, 4, 25969.	3.6	8
75	Forthâ€“back oscillated charge carrier motion in dynamically disordered hexathienocoronene molecules: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 17729-17738.	2.8	8
76	Adsorption of proline, hydroxyproline and glycine on anatase (001) surface: a first-principle study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	8
77	Theoretical Investigations on the Mechanism and Kinetics of OH Radical Initiated Reactions of Monochloroacetic Acid. Journal of Physical Chemistry A, 2017, 121, 6028-6035.	2.5	8
78	First principle studies on the atmospheric oxidation of HFC-C1436 initiated by the OH radical. New Journal of Chemistry, 2020, 44, 2070-2082.	2.8	8
79	Charge Transport and Optical Absorption Properties of Dibenzocoronene Tetracarboxdiimide Based Liquid Crystalline Molecules: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 3852-3862.	2.5	8
80	A quantative study of the charge-transfer between conjugated thiophene rings in vibrationally excited states. Physica B: Condensed Matter, 2004, 350, 220-223.	2.7	7
81	Theoretical investigation on intramolecular electron transfer in polypeptides. Chemical Physics Letters, 2007, 440, 302-307.	2.6	7
82	Low temperature method for synthesis of starch-capped ZnSe nanoparticles and its characterization studies. Journal of Applied Physics, 2012, 112, 114331.	2.5	7
83	Depletion of atmospheric ozone by nitrogen dioxide: a bifurcated reaction pathway. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	7
84	Reaction mechanism and kinetics of the degradation of bromoxynil initiated by OH radical. RSC Advances, 2014, 4, 7749.	3.6	7
85	Atmospheric oxidation mechanism of OH-initiated reactions of diethyl ether â€“ the fate of the 1-ethoxy ethoxy radical. RSC Advances, 2016, 6, 81354-81363.	3.6	7
86	Synthesis, structural characterization, DNA/protein binding and inÂvitro cytotoxicity of three structurally different organoruthenium metallates from single pot. Journal of Organometallic Chemistry, 2016, 825-826, 83-99.	1.8	7
87	Unimolecular decomposition of acetyl peroxy radical: a potential source of tropospheric ketene. Physical Chemistry Chemical Physics, 2020, 22, 26819-26827.	2.8	7
88	The influence of the shape and configuration of sensitizer molecules on the efficiency of DSSCs: a theoretical insight. RSC Advances, 2021, 11, 5556-5567.	3.6	7
89	Study of chemical bonding in H ₂ and HF molecules: Wave function and density functional theory (DFT) parameters approach. International Journal of Quantum Chemistry, 2000, 76, 662-669.	2.0	6
90	Effect of conformational degrees of freedom on the charge transfer in model tripeptide. Journal of Molecular Graphics and Modelling, 2009, 27, 784-791.	2.4	6

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91	Reaction mechanism and kinetics of the atmospheric oxidation of 1,4-thioxane by NO ₃ – A theoretical study. Canadian Journal of Chemistry, 2012, 90, 384-394.	1.1	6
92	Charge transport and optical properties of discotic liquid crystalline molecules THDDP and substituted THDP. International Journal of Quantum Chemistry, 2012, 112, 713-723.	2.0	6
93	A theoretical probe on the non-covalent interactions of sulfadoxine drug with pi-acceptors. Journal of Molecular Structure, 2014, 1074, 157-167.	3.6	6
94	Theoretical probe on modified organic dyes for high-performance dye-sensitised solar cell. Current Applied Physics, 2018, 18, 1071-1079.	2.4	6
95	Studies of chemical hardness and Fukui function using the exact solution of the density functional theory. International Journal of Quantum Chemistry, 2001, 81, 4-10.	2.0	5
96	A theoretical study on decomposition and rearrangement reaction mechanism of trichloroacetyl chloride (CCl ₃ COCl). International Journal of Quantum Chemistry, 2011, 111, 3482-3496.	2.0	5
97	Opto-electronic properties of low band gap fused-ring thieno[3,4-b]pyrazine analogues – A theoretical study. Molecular Physics, 2013, 111, 3036-3046.	1.7	5
98	Theoretical study on the gas phase reaction of methyl chavicol with hydroxyl radical. Computational and Theoretical Chemistry, 2019, 1151, 78-90.	2.5	5
99	Hydrolysis of HNSO ₂ : A potential route for atmospheric production of H ₂ SO ₄ and NH ₃ . International Journal of Quantum Chemistry, 2020, 120, e26182.	2.0	5
100	Reaction mechanism and kinetics of the degradation of terbacil initiated by OH radical – A theoretical study. Chemical Physics, 2018, 501, 110-120.	1.9	4
101	Mechanism and kinetics of the reaction of methyl acetate with Cl atom – A theoretical study. Computational and Theoretical Chemistry, 2018, 1131, 40-50.	2.5	4
102	Room temperature weakly ferromagnetic energy band opened graphene quantum dot coupled solid sheets – A possible carbon based dilute magnetic semiconductor. Applied Surface Science, 2021, 548, 149195.	6.1	4
103	Mechanism and kinetics of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical: a theoretical study. Structural Chemistry, 2014, 25, 1773-1783.	2.0	3
104	Adsorption of tetracyanoquinodimethane and tetrathiafulvalene on aluminium (100) surface – a first principle study of structural and electronic properties. Molecular Simulation, 2019, 45, 492-500.	2.0	3
105	Mechanism and kinetics of the oxidation of dimethyl carbonate by hydroxyl radical in the atmosphere. Environmental Science and Pollution Research, 2019, 26, 3357-3367.	5.3	3
106	Mechanism, Kinetics, and Ecotoxicity Assessment of •OH-Initiated Oxidation Reactions of Sulfoxaflo. Journal of Physical Chemistry A, 2021, 125, 10052-10064.	2.5	3
107	Modified fullerenes as acceptors in bulk heterojunction organic solar cells – a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 27468-27476.	2.8	3
108	Post Hartree-Fock and density functional theory studies on Di-Protonated Allopurinol ²⁺ . Computational and Theoretical Chemistry, 2007, 810, 25-30.	1.5	2

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109	Long-range charge transfer in donor-peptide bridge-acceptor model systems: A theoretical study. International Journal of Quantum Chemistry, 2011, 111, 3904-3914.	2.0	2
110	Adsorption of perfluoropentacene on aluminum (100) surface: Structural and electronic properties from first principle study. Computational Materials Science, 2014, 89, 216-223.	3.0	2
111	Counter anion effect on structural, opto-electronic and charge transport properties of fused π -conjugated imidazolium compound. Molecular Physics, 2018, 116, 1145-1152.	1.7	2
112	Theoretical Investigation on the Mechanism and Kinetics of Atmospheric Reaction of Methylchloroacetate with Hydroxyl Radical. Journal of Physical Chemistry A, 2018, 122, 9316-9325.	2.5	2
113	Molecular structure, conformational stability and cis effect of 1,4-dichlorobutadiene: a quantum chemical study. Computational and Theoretical Chemistry, 2002, 577, 69-79.	1.5	1
114	Conversion of toluene into benzyl radical on anatase TiO ₂ (0 0 1) surface. Computational and Theoretical Chemistry, 2017, 1115, 13-21.	2.5	1
115	Exploring the mechanisms for the radical induced damage of 6-thioguanine. International Journal of Quantum Chemistry, 2018, 118, e25544.	2.0	1
116	FOBEZ-256 (A hashing function using Bezier curve). , 2010, , .		0
117	Atmospheric oxidation mechanism and kinetics of 2-bromo-4,6-dinitroaniline by OH radicals: a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 21109-21127.	2.8	0
118	A comprehensive quantum chemical study on the mechanism and kinetics of atmospheric reactions of 3-chloro-2-methyl-1-propene with OH radical. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	0
119	Adsorption of phenanthroline and its derivatives on Au (111) surface: Influence of substitution on structure and electronic properties. Computational Materials Science, 2020, 182, 109778.	3.0	0
120	Crossover from static to dynamic Non-Condon effect on charge Transport in Organic Semiconductors. Journal of Physics: Conference Series, 2021, 1916, 012230.	0.4	0
121	Theoretical studies on adsorption of organic molecules on metal surface. , 2017, , 209-241.		0