



سه شنبه ۲۹ مرداد ۱۳۹۸، ساعت ۱۶:۰۰-۱۵:۳۰

(Computational Chemistry - Quantum Chemistry)

Poster No.	Paper Code	Presenter	Paper Title
1	IPCC22-1036	Maryam Ghaderi	Study of Methane, Ethane and Propane Adsorptions on ZJU-9a Using GCMC Method
2	IPCC22-1056	Rozbeh Azinfar	Synthesis and Investigation of Electrochemical Activity of Ni-Co/ poly (p-phenylenediamine) Catalyst Toward Methanol Electrooxidation
3	IPCC22-1126	Maede Zamani	Effect of 1,3:2,4-Bis (3,4-dimethylbenzylideno) Sorbitol as a Nucleating Agent on Crystallization of Poly (3-hydroxybutyric acid)
4	IPCC22-1097	Zahra Hasanzadeh Tazeh Gheshlagh	Electric Field Effect on the Adsorption of Li, Na, Mg and Ca on Silicene sheet: A DFT study
5	IPCC22-1100	Zahra Hasanzadeh Tazeh Gheshlagh	Quantum Capacitance Effect on silicene sheet doped with N, B and F atoms: A DFT study
6	IPCC22-1108	Nazila Golmohammadi	Structure and Dynamics in Poly(ethylene terephthalate): Coarse-Grained Molecular Dynamics Simulations
7	IPCC22-1107	Nazila Golmohammadi	Molecular Dynamics Simulation of Ionic Liquid 1-n-Butyl-3-Methylimidazolium Methylsulfate in Contact with a Silica Surface
8	IPCC22-1184	Negar Mehdizadeh darban	Study of the Structure of the Peptides Stabilized by the Hydrogen-Bond Surrogate Approach Using Molecular Dynamics Simulation
9	IPCC22-1306	Seyede Mahtab Hosseini	Hydrogen bonding in Systems Comprising Chitosan Nanoparticles/poly vinyl alcohol/Erythromycin
10	IPCC22-1249	Seyede Mahtab Hosseini	DFT Study Of Novel Drug Delivery Systems Comprising Nanoparticles Based On Chitosan Nanoparticles/Graphene Oxided/Folic Acide For Deliver Targeted Of The Chemotherapy Drugs
11	IPCC22-1234	Zahra Zarifnia	Study of adsorptions and separation of CO ₂ and H ₂ S in nanoporous carbon model by GCMC
12	IPCC22-1002	Tooba Afshari	DFT Studies of Ethylene Oxide Adsorption on Pristine and Ga-doped Carbon Nanotubes
13	IPCC22-1044	Maryam Aghilinategh	Direct Conversion Of Chlorella Vulgaris Microalgae To Biodiesel Under Supercritical Methanol Condition In The Presence of Heterogeneous Nano-photocatalyst
14	IPCC22-1085	Azadeh Daneshvar	The Effect of Cation Type and Temperature on the Transport Properties of Some Room Temperature Ionic Liquids
15	IPCC22-1086	Azadeh Daneshvar	A Quantum Study on the Fe-Containing Ionic Liquids
16	IPCC22-1083	Sogol Hajiyan	Investigation of the Heterogeneity Order Parameter of Four Different Imidazolium- And Cholinium-Based Ionic Liquids
17	IPCC22-1084	Sogol Hajiyan	Analysis of the Spatial and Radial Distribution Functions of Ionic Liquids with Different Cations
18	IPCC22-1048	Fariba Mohammadian-Sabet	Calculation of Electronic Spectra For Carbazole Derivatives For Applications in Thermally Activated Delayed Fluorescence
19	IPCC22-1183	Shahla . Heliche	Density Functional Study of two Heterodiazocine Molecular Photoswitches



20	IPCC22-1243	Shahla Heliche	Dispersion-Corrected Density Functional Study of two Acylhydrazone Molecular Photoswitches
21	IPCC22-1270	Samaneh baranipour	Molecular Dynamics Investigation of Gramicidin-C Peptide as antibacterial drug in DMPC Bilayers
22	IPCC22-1303	Parisa Jahanbakhsh-Bonab	Structural and Dynamical Properties of phenyl propanoic acid Via Molecular Dynamics Simulations
23	IPCC22-1031	Sahar Razzaghi	Studying Of Interaction Of Peptide Adsorbed On Graphene Using Molecular Dynamic Simulation
24	IPCC22-1156	Sahar Shokri	Molecular Dynamics Simulations of amino acid ionic liquids
25	IPCC22-1096	Leila Tohidifar	Preparation of Water Soluble Single Walled Carbon Nanotubes: Study of the Chirality Effect Insights from Molecular Dynamics Simulations
26	IPCC22-1102	Zohreh YOUSEFIAN	Investigation of N-doped Graphene as an absorbent for H ₂ S gas: A DFT Study
27	IPCC22-1189	Khadijeh Shekoohi	Theoretical Study of Oxime Derivatives containing Quinoxaline
28	IPCC22-1129	Marjan A. Rafiee	DFT Calculations of Iron Chelators as Siderophore Inhibitors
29	IPCC22-1130	Marjan A. Rafiee	DFT Calculations of Pressure Induced Phases of Calcium Borohydride as Hydrogen Storage Material in Fuel Cells
30	IPCC22-1032	Sara Fallah Ghasemi	Influence of various anions on physicochemical properties ionic liquids based on 1-benzy bis (1-2,3,4,6,7,8,9,10-octa hydroypyrimido [1,2-a] azepinium) dication: characterization and DFT calculations
31	IPCC22-1257	Maryam Dehestani	Theoretical investigation of inhibitors of HIV
32	IPCC22-1177	Maryam Dehestani	Effect of Silver Atom on Bis-GMA Structure: A Computational Chemistry Study
33	IPCC22-1092	Azar Larijani	QM study the inhibitory effect of Bisulfite Ion on inhibition of carbonic enzyme
34	IPCC22-1131	Azar Larijani	Comparison of the inhibitory effect of thiocyanate and isothiocyanate on inhibition of carbonic anhydrase enzyme: The DFT study
35	IPCC22-1106	Hamideh Basouli	Molecular Dynamics Simulation of Ionic Liquid 1-Ethyl-3-Methyl Imidazolium Methyl Sulfate
36	IPCC22-1244	Hossein Mohammadi-Manesh	Thermal Expansion Coefficient of sI Clathrate Hydrates by Molecular Dynamics Simulation
37	IPCC22-1289	Mina Amiri	investigation of thermal decomposition and chemical ionization of N-aminophthalimide in the gas phase using ion mobility spectrometry
38	IPCC22-1269	Nasibeh Dehghani	Theoretical investigations of copper ion selectivity by new fluorescent chemo sensor based on carbazole-Schiff
39	IPCC22-1253	Babak Mirtamizdoust	DFT Calculations and Theoretical Investigations of an innovative Lead(II)-nitrite metal-ligand compound
40	IPCC22-1091	Seyedeh Shabnam Daryabari	Electric Field Effect on the Interaction of Helium with Defected Graphene Sheet: A DFT Study
41	IPCC22-1090	Seyedeh Shabnam Daryabari	Separation and Diffusion of Helium from Defective Graphene A comparative DFT study



42	IPCC22-1028	Samira Gholami	Theoretical Study of Carbonic Anhydrase Inhibition by natural products
43	IPCC22-1137	Vahideh Pourghasem	Interaction of Polyphenols with Nerve Growth Factor: A Docking Studies
44	IPCC22-1144	Hadi Hamid	QTAIM study of a single molecular wire: Quantum atomic-scale study
45	IPCC22-1059	Neda Najjari Milani	Theoretical investigation of vinylogous anomeric effects on the stability of 4-H-4-amino-1-methylpyridin and its analogues
46	IPCC22-1060	Neda Najjari Milani	Theoretical research of vinylogous Anomeric effects on the stability of 4-H-4-triazole-1-methylpyridin and its analogues
47	IPCC22-1081	Maryam Yousefizadeh	(Computational assessment of the electro-optical characteristics of Lin@B12 (n=1, 2, 3
48	IPCC22-1314	Zahra Tohidi Nafe	DFT Calculation of the Enol Content of Acetone in the Presence of Water Clusters
49	IPCC22-1121	Farideh Salari	QM Study of complex between Acetazolamide inhibitor and human α -carbonic anhydrase enzyme
50	IPCC22-1205	Esmail Sanchoo	Exploring binding of some 4H-benzo[g][1,2,3]triazolo[5,1-c][1,4]oxazocine derivatives with calf thymus DNA using computational methods
51	IPCC22-1138	Marzieh Rafiee	Kinetic Monte Carlo Simulation of hydrogen production from formic acid decomposition on Cu(100) catalyst
52	IPCC22-1049	Marzieh Sarafrazia	Surface interaction energy simulation of TiO ₂ and SiO ₂ -TiO ₂ layers with Epoxy resin
53	IPCC22-1272	Mohammad Kowsari	Molecular Dynamics Simulation of Aqueous Solutions of a Hydrophilic Room Temperature Ionic Liquid
54	IPCC22-1133	Ali reza Shayesteh	Rotational and Spin-Orbit Hamiltonian Matrices for Low-Lying States of NiH
55	IPCC22-1034	Tahereh Lotfi	The Influence of Li Atoms on Electronic and Structural Properties of Silicon Carbide Nano sheets.
56	IPCC22-1033	HosainNikoofard	Density Functional Theory Study on the Oxidation Reaction of 3-Phenylthiophen Derivatives
57	IPCC22-1178	Ghazaleh Gharajeh Marand	The role of internuclear distances in the minima and electron states in HHG of H ₂ ⁺
58	IPCC22-1192	Zahra Safari	Photophysical Properties of Thermally Activated Delayed Fluorescence Emitters From Optimally Tuned Range-Separated Functionals
59	IPCC22-1212	Mahnaz Jabbarzadeh Sani	Spin-Orbit Coupling Effect on the Electronic Properties of Neutral Gold Clusters
60	IPCC22-1248	Nasibeh Tavakoli	Theoretical study of adsorption of trichloroethylene on the surface of beryllium oxide nanotubes
61	IPCC22-1016	Maryam Nayebzadeh	The studies of kinetic and atmospheric reaction mechanisms of pyrene in the presence of OH radicals
62	IPCC22-1176	Nazli Morovati	Wettability of Electrochemically Activated Carbon Cloth
63	IPCC22-1191	Nazli Morovati	Efficient electrocatalytic hydrogen evolution reaction on MoS ₂ nanosheets coated carbon cloth
64	IPCC22-1123	Atefeh Akbarnia Dafrazi	Dielectric study of 1,3 and 1,4-butandiol and cyclopentanone



چهارشنبه صبح ۳۰ مرداد ۱۳۹۸، ساعت ۱۱:۰۰-۱۰:۳۰

(Chemical Thermodynamics - Chemical Kinetics - Statistical Thermodynamics)

Poster No.	Paper Code	Presenter	Paper Title
1	IPCC22-1159	Nosaibah Ebrahimi	Salting Effect of Amino Acids and Surfactants on the Clouding Behavior of Polypropylene Glycol in Aqueous Media
2	IPCC22-1182	Shadieh Yadollahzadeh	Volumetric and Compressibility Studies of Tetraalkylammonium Bromide Salts in Aqueous Solutions at Different Temperatures
3	IPCC22-1233	Saeid Faraji	Prigogine-Flory-Patterson theory to correlate the excess molar volume and study of interactions for aqueous solutions of some choline chloride based deep eutectic solvents
4	IPCC22-1079	Fatemeh Sayyadi-Kalashami	Thermodynamic Study of (CaCl ₂ + N,N-Dimethylacetamide + H ₂ O) System Based on Potentiometric Measurements at T = 298.2 K
5	IPCC22-1265	Masumeh Mokhtarpour	Correlation of Celecoxib Solubility in Aqueous Solutions Containing Some Choline Based Deep Eutectic Solvents as Sustainable Solvents
6	IPCC22-1149	Asma Sadr-Mousavi	Thermodynamic Behaviour Of Lithium Chloride Solutions Containing Deep Eutectic Solvent In The Dilute Region At T = (288.15 to 303.15) K
7	IPCC22-1172	Fatemeh Pasham	Determination of Kamlet-Abboud-Taft solvatochromic parameters in some green solvent mixtures
8	IPCC22-1225	Hemayat Shekaari	Effect of choline chloride/urea deep eutectic solvent as green and sustainable solvents on conductivity of aqueous sugar solutions
9	IPCC22-1227	Selva Golgoun	Study of molecular interactions between choline chloride/urea deep eutectic solvent and meloxicam
10	IPCC22-1155	Vahideh Masumi	. Gibbs energies of transfer of NH ₄ SCN from water to aqueous solution of Butanol using Potentiometric Method
11	IPCC22-1152	Negin Ammari	Volumetric Properties of Ternary Mixtures for Choline Salicylate (API-IL) + Amino acids + Water at T = 298.15 K
12	IPCC22-1094	Fatemeh Parviz	Volumetric and electromagnetic study of the binary mixtures nonelectrolyte solutions dibutylamine /1-heptanol at different temperatures
13	IPCC22-1173	Yeganeh Nachari	Study on the protonation equilibria of drug naproxen in different surfactant media
14	IPCC22-1190	Maryam Abedi	Prediction of Water Content in Poly (Para-Phenylene terephthalamide) Based on Non-Electrolyte Flory-Huggins Theory
15	IPCC22-1140	Maryam Abedi	Determination of Ion Activity Coefficients in Aqueous Solutions of Mixed Electrolyte with a Common Ion: NaNO ₃ + NH ₄ NO ₃ , NH ₄ Cl + LiCl and KBr + KCl
16	IPCC22-1050	Haheh Ghazipour	Measurement the Sound Speeds, Densities and Refractive Indices of Biodiesel Components and Their Alcoholic



			Mixtures with 2Methyl1butanol, 2Butanol and 1,2Butandiol
17	IPCC22-1052	Haleh Ghazipour	An Experimental Approach to the Surface Properties of Biodiesel Components and Their Mixtures with Some Alcohols
18	IPCC22-1026	Sanaz Haghgoo	Electrophilic and Nucleophilic Activities of C40N20 and C42N18, a DFT Study
19	IPCC22-1027	Sanaz Haghgoo	Theoretical Study on the Absorption of some Metal Oxides on Fullerene C60 as Potential Detectors for NO2
20	IPCC22-1148	Elnaz Pourbagherian	Study of the liquid-liquid equilibrium for aqueous systems containing choline bitartrate and 1-propanol at different temperatures and their performances in acetaminophen separation
21	IPCC22-1238	Mehdi Dadkhah Tehrani	Experimental study on the calorimetric data of Aniline + Alkylamine (C4 and C6) at 303.15 K.
22	IPCC22-1087	Mostafa Rajabzadeh	Investigation of changes effect of glycine / urea ratio on ΔC_p during the process of synthesis of alumina nanopowder
23	IPCC22-1019	Mohammad Tashakori	Solvent Effects in the Reduction of Hydrogen Peroxide in presence of Glutathione Peroxidase Mimic, Molecular Approach
24	IPCC22-1236	Hadi Zarepour	The gas phase reaction of $CH_2CH_2OH + NH_2$: A computational study
25	IPCC22-1237	Hadi Zarepour	The reaction of $CH_2OH + 3NH_2$ in the gas phase
26	IPCC22-1042	Rahman Padash	Kinetics of chemical equilibrium between adenine and its tautomers
27	IPCC22-1120	Rahman Padash	Dynamic and Kinetic Parameters of $NH_2 + "H"_{-}2$ Reaction on an Interpolated Potential Energy Surface
28	IPCC22-1061	Ali Mehrizad	Adsorption study of Penicillin onto Single-Walled Carbon Nanotubes from Kinetics Perspective
29	IPCC22-1068	Ali Mehrizad	Photocatalytic Degradation of Direct Blue 14 by Polyaniline/CdS Nanocomposite
30	IPCC22-1020	Roghaieh Maghbool	Electro-Fenton-like process for treatment of aqueous solution of MO dye
31	IPCC22-1022	Elham Vesali-Kermani	Photofixation of Dinitrogen to Ammonia by ZnO Nanostructure Decorated with MnV_2O_6 under Ambient Conditions
32	IPCC22-1024	Soheila Asadzadeh-Khaneghah	g-C3N4 nanosheet/Carbon dots/BiOBr Nanocomposite: An Impressive Photocatalyst for Degradation of Congo-Red Dye Under Visible-Light Illumination
33	IPCC22-1104	Raziyeh Sharafdini	Collision Processes, Dynamic Parameters, Temperature Dependence of the Collisional Rate Coefficients of $NH_2 + OH$ and Deuterated Analogues on an Interpolated Potential Energy Surface



34	IPCC22-1105	Raziyeh Sharafdini	Theoretical Dynamics Study of Cytosine Tautomerism in the Gas Phase and Interaction of Na ⁺ With Its Tautomers
35	IPCC22-1195	Hamid Arjmandfar	The Potential Energy surface of Numan Rotation of N,N'-dinitrosopiperazine: A Theoretical study
36	IPCC22-1194	Hamid Arjmandfar	Theoretical study on the Potential energy surface of Numan rotation of N-Nitrosopiperazine
37	IPCC22-1235	Mohammad Kazemian	One-Pot Synthesis of Succinimide-3-Carboxamide Derivatives Using Microwave and Mechanistic insights and Kinetics analysis by Computational Method
38	IPCC22-1294	Maryam Noori	Kinetic Studies of Oxidative Addition Reaction of Ethyl Iodide for Synthesizing New Pt(IV) Complex
39	IPCC22-1295	Maryam Noori	Investigation of DNA Interaction with Two New Platinum(II) Complexes
40	IPCC22-1239	Khadigeh Seydi	The effect of water on the HS + HOCl reaction: mechanistic and thermodynamic viewpoints
41	IPCC22-1240	Khadigeh Seydi	The atmospheric reaction of HS + HOCl: mechanistic and thermodynamic viewpoints
42	IPCC22-1113	Narges Ghaderi	Isotherm and Kinetic Studies of the Bi(III) Extraction from Hydrochloric Acid Media by a Polymer Inclusion Membrane Containing Trioctylamine
43	IPCC22-1023	Solmaz Feizpoor	High efficient photocatalytic degradation of Malachite green using visible-light- driven TiO ₂ /CDs/Polyaniline photocatalyst
44	IPCC22-1165	Somayeh Rezheh	Starch-poly(acrylic acid)-Cu(II) Based Catalyst for Kinetic Studies in Epinephrine Oxidation
45	IPCC22-1164	Somayeh Rezheh	P(AA)-Co(II) Based Catalyst for Kinetic Studies in Methyl Orange Degradation
46	IPCC22-1021	Mina Sabri	Persulfate ions activated TiO ₂ /Carbon dots nanocomposite as a highly active photocatalyst for the degradation of Congo red under visible-light illumination
47	IPCC22-1101	Parvin Gharbani	Study of Reactive Yellow 145 Removal by Ag/GO nanocomposite using Response Surface Methodology
48	IPCC22-1098	Parvin Gharbani	Equilibrium and Kinetic Study of 4-Nitrophenol Removal by Modified Silk Waste
49	IPCC22-1132	Salar Bahrami	Kinetic and Isotherm Modeling Studies of the V(V) Extraction from Sulfate Solution Using an Aliquat® 336/PVDF-Co-HFP Polymer Inclusion Membrane
50	IPCC22-1115	Hadiseh Asgari	Corresponding States Correlations for Viscosity of Dilute n-Butane
51	IPCC22-1170	S.A. M Mirsaeidi	Using Artificial Neural Network For Modeling of Thermophysical Properties Of Carbon Quantum Dot based nanofluids
52	IPCC22-1208	S.A. M Mirsaeidi	Excess Molar Volume of Ternary System of Ionic Liquids Using Artificial Neural Network
53	IPCC22-1220	Azim Soltanabadi	Experimental and Computational Studies of Binary Mixtures of Morpholine + Cis and Trans 2-Methylcyclohexanol



54	IPCC22-1290	Azim Soltanabadi	Molecular Dynamics Simulations of the Structure the Graphene–Dicationic Ionic liquid interface
55	IPCC22-1114	Shirin Karimi	Viscosity of Ethane at Low and Moderate Densities Using Corresponding States Correlations
56	IPCC22-1051	Azita Amouzad Khaliliaa	Molecular simulations adsorption of hydrogen sulfide, carbon dioxide, methane and nitrogen and separation of binary mixtures (H ₂ S/CH ₄), (CO ₂ /CH ₄) into NUM-3a metal–organic frameworks
57	IPCC22-1247	Khadigeh Kazemi	Mathematical modeling of liquid phase equilibria for the systems (water + phosphoric acid + linear alcohols) using the GMDH-type neural network
58	IPCC22-1309	Maryam Kamal Kandezi	Selective Ion Separation Using B-N Doped Graphene Sheet
59	IPCC22-1310	Maryam Kamal Kandezi	Calculation Young moduli for B-N doped and undoped graphene sheet
60	IPCC22-1297	Tahereh Daneshdar	Measuring and Modeling of Thermodynamic Properties of Alkanol Amin
61	IPCC22-1179	Maryam Kebriaei Amjad	Densities and derived thermodynamic properties study for the binary mixtures of (Ethyl methyl ketone, N,N-Dimethylbenzylamine) at different temperature
62	IPCC22-1230	Negar Oliya	Effect of choline lactate as novel green solvent on the aqueous solubility of acetaminopehn
63	IPCC22-1317	Mahdi Ziaee	Investigation on the Mutual Interplay between the Physicochemical Properties of 1-octyl-3-Methylimidazolium Bromide, [C8mim][Br], and CuO Nanofluids by Measuring the Electrical Conductivity, Surface Tension ,and Static Contact Angle



عصر چهارشنبه ۳۰ مرداد ۱۳۹۸، ساعت ۱۶:۰۰-۱۵:۳۰

(Chemistry Engineering-Polymer Physics Chemistry-Polymer Chemistry Chemistry- Applied-Electrochemistry-Surface Chemistry Chemistry-Experimental Spectroscopy)

Poster No.	Paper Code	Presenter	Paper Title
1	IPCC22-1241	Maryam Shahabi	New Insight into Ice Growth and Inhibition by Antifreeze Protein: Atomistic Molecular Dynamics Simulation
2	IPCC22-1069	Mohammad Firouz	The Mathematical Modeling of Open Cooling Tower and the Effect of Air Humidity on Outlet Water Temperature
3	IPCC22-1072	Mona Nabizad Gharani	Adsorption of cefixime from aqueous solution using Fenton process in presence of nanostructured magnetic alginate composite and nanostructured alginate-hydroxyapatite composite
4	IPCC22-1145	Navvab Zamani Nejad	Comparison of the performance of chemical demulsifiers in the separation of water emulsions in Iranian heavy crude oils
5	IPCC22-1103	Ardashir Hassanzadeh	Investigation of Carbon Dioxide and Hydrogen Sorption in ZSM-5 Using Grand Canonical Monte Carlo Simulation
6	IPCC22-1055	Fatemeh Sabzi	Thermodynamic Modeling of Hydrogen Solubility in [MDEA][Cl] Using Sanchez-Lacombe Equation of State
7	IPCC22-1099	Fatemeh Sabzi	Solubility of Hydrogen Sulfide in 1-ethyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate
8	IPCC22-1160	Leila Ebrahimi	Development of Optimized Potentials for Liquid Simulation All-Atom (OPLS-AA) Force Field to Sarin Nerve Agent
9	IPCC22-1057	Zahra Soudi	Removal of Direct Red Photocatalytic under Visible Light Radiation by Magnetic Spinel CoFe ₂ O ₄
10	IPCC22-1058	Zahra Soudi	Synthesis of Magnetic Spinel CoFe ₂ O ₄ by Hydrothermal Method and Study of Photocatalytic Activity
11	IPCC22-1274	Javad Azizi	Enhancement electrochemical activity of Pt nanoparticles toward methanol oxidation by using a new substrate
12	IPCC22-1273	Javad Azizi	Synthesize of bimetallic nanocomposite on the polymeric substrate for the electrochemical oxidation of methanol
13	IPCC22-1166	Mahdi Cheraghi Iranshahi	Physical Properties of the Pseudo-Ternary System of Deep Eutectic Solvent (Choline Chloride+ Glucose) + K ₂ HPO ₄ + Water
14	IPCC22-1014	Elham Norouzi	Physical Properties of Choline chloride+K ₃ PO ₄ +H ₂ O System
15	IPCC22-1283	Zahra Alipour	Nanocomposite Decorated Glassy Carbon Electrode for Simultaneous Determination of Dopamine and Uric acid
16	IPCC22-1299	Zahra Alipour	ZnO Nanoparticles Anchored 3-D Ni-Foam Electrode for Electrochemiluminescence Determination of Amoxicillin
17	IPCC22-1286	Fatemeh Zandiyan	Electrochemical Behavior Study of Flutamide in Aqueous Solutions
18	IPCC22-1185	Amaneh Amani	Experimental and Theoretical Analysis of the Electrochemical Oxidation of 3,4-Dihydroxy-Cinnamic Acid in the Presence of 2-Mercaptobenzimidazole

19	IPCC22-1198	Gholam reza Allahgholipour	Corrosion Behavior of Electrodeposited Ni-W-P-SiO ₂ Nanocomposite Coatings in NaCl Solution
20	IPCC22-1151	Tohid Khanahmadlou	Wireless Photoelectrochemical Degradation of Methylene Blue Dye Using a NiCo ₂ O ₄ /Cu Photoelectrode
21	IPCC22-1008	Mahsa Ghasemi	Ion-ion and ion-solvent interaction studies on the ternary system: KSalicylate+ Ethanol+ H ₂ O by Potentiometric Method
22	IPCC22-1029	Faezeh Shirzadi	Diversity of mechanism in the electrochemical study of different electrophiles in the presence of some thiol nucleophiles: thermodynamic and mechanistic study
23	IPCC22-1015	Shadi Paziresh	Experimental and computational study of the electrochemical oxidation of some urazole species
24	IPCC22-1262	Somayeh Majidi	Long-Term Activity of Pd-Co/rGO Nano-Catalyst in Ethylene Glycol Electro-oxidation Reaction in Alkaline Media
25	IPCC22-1030	Faezeh Shirzadi	Electrochemical oxidation of some hydroquinone derivatives in the presence of p-toluenesulfonic acid: Thermodynamic and Mechanistic studies
26	IPCC22-1073	Faranak Haghani Dogahe	Thermodynamic Study of 1-Butyl-3-Methylimidazolium Bromide Ionic Liquid In Water + DMA Mixtures Based On Conductometric Measurements
27	IPCC22-1007	Parisa Ghasemi	An investigation on specific conductivities of the ternary KCl-[C ₆ mim][Cl]-H ₂ O system using semi-ideal solution theory at 298.15 K
28	IPCC22-1229	Roghaieh Mohammadi	Synthesize and Electrocatalytic Investigation of CuFe ₂ O ₄ Nanostructures
29	IPCC22-1193	J. Nazari	Application of Electroless nickel plating on AM60B magnesium alloy via Ti-Zr/sol-gel composite layer as a pretreatment
30	IPCC22-1232	Alieh Babaei	Sol-gel auto-combustion synthesis of SnO ₂ Nanopowders: Application in Electrochemical Studies
31	IPCC22-1150	Jaleh Nazari	Studying the Effect of Nitric Acid on the Physical Chemistry Properties of the Prepared Extrudates Catalyst Support from Boehmite Powder of Nephleensinite Ore Mines
32	IPCC22-1251	Hossein Tajabadipour	Investigating the Effect of Pantoaprazole for Corrosion Protection of Mild Steel
33	IPCC22-1278	Mohammad Rafi	Mechanism of Adsorption of Congo Red on the Surface of Filter Paper in NaCl and 2-propanol Solutions
34	IPCC22-1280	Mohammad Rafi	Silica Gel Dyeing by Adsorption of a Series of Triphenylmethane Dyes on its Surface
35	IPCC22-1298	Javad Adabi Firuozaie	Study of optical energy gap of AL-doped ZnO ₂ nanoparticles synthesized by sol-gel method
36	IPCC22-1054	Ghazaleh Kouchakzadeh	Application of Persimmon Tree Leaf for Dye Removal
37	IPCC22-1304	Ensiyeh Shabanlu	The Effect of Laser Polishing on Titanium Surface in Nitrogen Media



38	IPCC22-1258	Mohammad Ali Rezvani	Synthesis of new nanocomposite vanadium containing phosphomolybdovanadate / polyvinyl alcohol as a nanocatalyst for germination of barley seeds
39	IPCC22-1005	Seyed Mohsen Mahdavi Abandansari	Study of optical energy gap of Ag-doped ZrO ₂ nanoparticles synthesized by sol-gel method
40	IPCC22-1010	Aida Ghary Haghghat	The Effect of Urea on Aggregation Properties of Methylene Violet Dye
41	IPCC22-1045	Tayyebe Nosrati Fallahkar	Conductometric Study of 1-Propyl-3-methylimidazolium Bromide Ionic Liquid in Water and Ethylene Carbonate Mixtures
42	IPCC22-1035	Taibeh Rostami	The Investigation of Thermal Conversion of Spiropyran to Merocyanine and its Derivatives
43	IPCC22-1282	Fahimeh Khouini	Chemical Ionization of Thiosemicarbazide; Ion Mobility Spectrometry and Theoretical Calculations
44	IPCC22-1197	Masoumeh Ghahremani	Investigation of Gas Phase Protonation of 2-Mercaptobenzothiazole; Ion Mobility Spectrometry and DFT calculations
45	IPCC22-1315	Masoumeh Ghahremani	Chemical Ionization of Barbituric acid in Corona discharge
46	IPCC22-1281	Mahsa Yousefian	Experimental and Theoretical Investigation of 5-aminoindole Chemical Ionization
47	IPCC22-1089	Peyman Mohammadzadeh Jahani	Theoretical study of intramolecular hydrogen bond on 2-(2-Hydroxy phenyl)-5(4H)-Oxazolone halogenated derivatives in ground state
48	IPCC22-1064	Zohreh Malek Esfandiyari	Multi-spectroscopy of the interaction behavior between calf thymus DNA and Rebecamycin in binary and ternary approaches
49	IPCC22-1065	Zohreh Malek Esfandiyaria	Spectroscopic studies on the interaction of Rebecamycin with calf thymus DNA in the absence and presence of Histone H1
50	IPCC22-1293	BaharehNorouzneh zhad	Biochemical Studies of A New Schiff Base Ligand and Its Complex Containing 2-Thiophenecarboxaldehyde
51	IPCC22-1157	Azam Shiri	Substitution effects on philicity of 1,3-diarylphosphole-2-ylidenes based on DFT method
52	IPCC22-1287	Siavash Jami	Optimization of deposition voltage for copper electrodeposition on FTO from non-acidic solution
53	IPCC22-1279	Saleh fallah samakosh	Study and investigation TCTA as a hole transport layer in the organic light-emitting diode
54	IPCC22-1167	Leily Heidarpoor Saremi	Pterostilbene: a Theoretical Elucidation on Its Antioxidant Activity
55	IPCC22-1312	Elmira Ghazanfari jajin	Numerical Investigation Effect of Geometry in Micro Droplet Generation
56	IPCC22-1318	Muhammad reza Zarifiyan	Protonation of Gabapentin, ab initio study
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60	IPCC22-1119	Niloufar Foghahazade	A Novel ZnO/BiFeO ₃ Photocatalyst for Highly Efficient Visible Photocatalytic Performance
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زمان بندی ارائه مقالات پذیرفته شده به صورت پوستر



Haghani

Hexylethylenediaminium Trifluoromethanesulfonate



پنجشنبه صبح ۳۱ مرداد ۱۳۹۸، ساعت ۱۱:۰۰-۱۰:۳۰

(Physics biochemistry-drug computational design-bio-physics chemistry-education-nano-chemistry-nano-computing)

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1	IPCC22-1125	Hujjat Delarami	Antibacterial evaluation of some synthetic thiazole compounds using the molecular docking study
2	IPCC22-1124	Hujjat Delarami	Anticancer Activity Evaluation of Some 1-hydroxynaphthalene-2-carboxanilide Derivatives Using the Computational Methods
3	IPCC22-1077	Elaheh Mousavi	Docking and virtual screening for determination of new derivatives of anti-cancer drugs from quinazoline compounds
4	IPCC22-1218	Marzieh Ajamgard	Computational Study of the Inhibition of HIV-1 Protease by RNA Aptamer: Effect of the Form of Dimer and Monomer in Protease
5	IPCC22-1222	Somayya Shahraki	Effects Of Isoxsuprine On The Catalytic Activity Of Catalase. Kinetics, Interaction Mechanism And Molecular Docking Approach
6	IPCC22-1224	Somayya Shahraki	Molecular Docking And Analysis Of Binding Interaction Between Levothyroxine And Bovine Liver Catalase
7	IPCC22-1210	Nafiseh salehi	Novel p21-Activated Kinase 4 (PAK4) and an effective in vitro inhibitor
8	IPCC22-1039	Razieh Habibpour	Evaluating Dopamine Targeting Drugs for Treatment of Schizophrenia By Applying a Practical Java Tool
9	IPCC22-1040	Razieh Habibpour	Generating the Supplementary Structure of Dopamine D2 Receptor Based on the X-ray Crystal Structure for Molecular Modeling
10	IPCC22-1291	Sanaz Kaveian	Endohedral and Exohedral adsorption of helium on X ₁₂ N ₁₂ (X = B, Al) nano-cluster: A DFT study
11	IPCC22-1292	Sanaz Kaveian	Theoretical study on Solubility of vitamin C-adsorbed carbon nanotube and graphene in some organic solvents
12	IPCC22-1047	Raheleh Rahbar Kahkha	Studying the interaction of phosphodiesterase inhibitors in the treatment of Alzheimer's disease
13	IPCC22-1162	Marzieh Moeeni	Interaction of Superparamagnetic Iron Oxide Nanoparticles with Bovine Alpha-Lactalbumin
14	IPCC22-1088	Afsaneh Askari	Spectroscopic Study of the Interaction of Trans_Aco Base (curcuminato) Exo Zirconium IV Hydrate and Curcumin with Bovine Serum Albumin
15	IPCC22-1242	Mojgan Biuki	Spectroscopic Study of the Interaction of Trans_Aco Base (curcuminato) Exo Zirconium IV Hydrate and Curcumin with DNA
16	IPCC22-1082	Zahra Shabanzade	Spectroscopic Study of the Interaction of Trans Aco Base (curcuminato) Exo Zirconium IV Hydrate and Curcumin with Human Serum Albumin
17	IPCC22-1168	Maryam Ghorbani	Effect of different concentrations of 1-Butyl-3-methylimidazolium bromide on activity and structure of Chloroperoxidase: Molecular Dynamics Simulation
18	IPCC22-1202	Hossein	Selective sensing of Fe ³⁺ and Al ³⁺ over mixed metal ions using



19	IPCC22-1186	Shayegan Hassan Faridnouri	functionalized microporous MOF as a new fluorescent probe Thermal stability improvement of tyrosinase in the presence of spermine
20	IPCC22-1226	Samira Seyed Somarin	Direct electron transfers study of immobilized tyrosinase using the modified glassy carbon electrode by MWCNT/ poly (aniline-co-metha phenylene diamine) composite
21	IPCC22-1095	Samaneh Shakeri	Binding interaction of disperse azo dye with bovin serum albumin by spectroscopic techniques
22	IPCC22-1277	Negar Parvizi	Insights into the Binding of Cafaminol to Human Serum Albumin: Multi-Spectroscopic and Molecular Modeling Studies
23	IPCC22-1154	Amaneh Amani	Electrochemical Evaluation of Antioxidant Activity and Herb-Herb Interaction of Iranian Echium amoenum Fisch and Citrus aurantifolia aqueous extracts
24	IPCC22-1209	Fatemeh Fateminasab	Inclusion Complexes between (α -, β - and γ -) cyclodextrins as a nanocarriers with serotonin: Molecular Docking and Molecular Dynamics simulation
25	IPCC22-1228	Mehrdad Bamdad	Thermal Efficiency for a Curzon and Ahlborn Engine
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28	IPCC22-1263	Farshad Mirzaee	Novel Cu ₂ O/Cu-MOF/rGO is reported as Highly Efficient Catalyst for Reduction of 4-Nitrophenol
29	IPCC22-1264	Farshad Mirzaee	Noble Metal Nanoparticles Supported on Ni Promoted MoS ₂ as an Efficient Catalyst for p-Nitrophenol Reduction
30	IPCC22-1070	Amin Norouzi	Fabrication and Investigation of an Easy-to-Prepare Highly Sensitive Temperature Sensor Based on Epoxy Resin/Copper (II) Oxide Nanoparticles/ MWCNTs Nanocomposite
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32	IPCC22-1276	Masomeh Rahmati	Application of MCM-41/CuO for Oil Pollutions Treatment: Optimization Process Based on Taguchi Design Method
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34	IPCC22-1066	Sara Naseh	Unexpected Electronic and Conductive Properties of Aniline/CONH ₂ -SWCNT Binary Nano-combination for Use as Counter Electrode
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36	IPCC22-1296	Zahra.Kavianfar	Exploring the effect of surface functionalization of superparamagnetic iron oxide nanoparticles (Fe ₃ O ₄) on the interaction with BLG
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45	IPCC22-1046	Soha Shamae	Titanium decorated graphdiyne as a hydrogen storage medium
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47	IPCC22-1143	Hossein Mostaanzadeh	DFT Investigation of Inhibitive Behaviour of Some Phenylurea Derivatives on Steel corrosion
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50	IPCC22-1266	Masomeh Keyhanian	The adsorption behaviors of phenol on the surfaces of pristine and M-encapsulated B38 borofullerene: DFT investigation
51	IPCC22-1246	Masomeh Keyhanian	A theoretical investigation on interaction of deposited B38 borofullerene on bowl-shaped B36 cluster
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58	IPCC22-1316	Maryam Shaterian	Synthesize, Characterization and Band Gap Calculation of Zinc Ferrite Nanostructures