«باسمه تعالی»

برنامه و جدول زمانی **کنفرانس نانو محاسباتی** دانشگاه آزاد اسلامی واحد علوم دارویی ۲۷ بهمن ۱۳۹۱

CONFERENCE OF NANO COMPUTATIONS (Feb. 15, 2013) http://CNC.iaups.ac.ir

۷:۳۰ – ۸:۳۰	پذیرش (لطفاً کارت ملی و اصل فیش واریزی وجه ثبت نام را همراه داشته باشید)
۸:۳۰ – ۹:۰۰	مراسم افتتاحیه کنفرانس
۹:۰۰ – ۱۰:۱۰	سخنرانی اساتید مدعو
۱۰:۱۰ – ۱۰:۳۰	استراحت و پذیرایی
۱۰:۳۰ – ۱۲:۳۰	ارایه مقاله شرکت کنندگان به صورت سخنرانی در سه پانل موازی – جلسه صبح (به صفحات ۲ الی ۵ مراجعه شود)
۱۲:۳۰ – ۱۳:۳۰	نماز و نهار
۱۳:۳۰ – ۱۵:۰۰	ارایه مقاله شرکت کنندگان به صورت پوستر (به صفحات ۶ الی ۱۲ مراجعه شود)
۱۵:۰۰ – ۱۷:۱۵	ارایه مقاله شرکت کنندگان به صورت سخنرانی در سه پانل موازی – جلسه عصر (به صفحات ۲ الی ۵ مراجعه شود)
۱۷:۱۵ – ۱۸:۰۰	مراسم اختتامیه کنفرانس

آدرس دقیق محل برگزاری: تهران، خیابان دکتر شریعتی، قُلهَک، ابتدای خیابان یخچال، دانشگاه آزاد اسلامی واحد علوم دارویی، دانشکده داروسازی

بهترین راه دسترسی: خط ۱ مترو، ایستگاه متروی قُلهَک تلفن: ۵ – ۲۲۶۴۰۰۵۱ (۰۲۱)

فهرست مقالات برای ارایه به صورت سخنرانی در کنفرانس نانو محاسباتی دانشگاه آزاد اسلامی واحد علوم دارویی ۲۷ بهمن ۱۳۹۱

۱- لطفاً New Code را برای مقاله خود به خاطر بسپارید، تعیین پانل ها بر اساس New Code خواهد بود

۲- ارایه مقالات در سه پانل موازی و هر پانل در دو جلسه صبح و عصر صورت می گیرد، جلسه صبح از ساعت ۱۰:۳۰ الی ۱۲:۳۰ و جلسه عصر از ساعت ۱۵:۰۰ الی ۱۷:۱۵

۳- در تهیه اسلایدهای سخنرانی، به تعداد مطلوب اسلاید برای کنفرانس توجه فرمایید (۱۲ اسلاید برای ۱۲ دقیقه)، خواهشمند است از مقدمه گویی در اسلایدها پرهیز فرمایید و تمرکز را در ارایه مقاله روی کار انجام شده توسط محقق / گروه محققین بنا نهید

۴- زبان مورد استفاده در تهیه اسلایدها دلخواه است

۵- در صورت ارایه سخنرانی، گواهی ارایه مقاله صادر می شود

فهرست مقالات برای ارایه به صورت سخنرانی در **کنفرانس نانو محاسباتی** دانشگاه آزاد اسلامی واحد علوم دارویی ۲۷ بهمن ۱۳۹۱

New Code	Old Code	Title of Oral – Panel 1: Quantum Computations	Presented by	Time
OP101	OA101	A theoretical study of functionalized single-wall carbon nanotubes by ONIOM calculations	Shamshiri, M.	10:30
OP102	OA104	DFT study of the Germanium Nitride and Boron Nitride Nanocages	Vafaei, H.	10:45
OP103	OA112	Square- and Hexa-Cross sectional Carbon and Boron-Nitride Nanoneedles	Salehfar, S.	11:00
OP104	OA119	A comparative study of methane molecule adsorption onto graphene and white graphene sheet	Seyed Talebi, S.M.	11:15
OP105	OA114	Electronic Investigation of Boron-Nitride Nano-Flakes	Nejati, A.	11:30
OP106	OA117	Study of gas absorption in BN-doped single-walled carbon nanotubes: A computational NMR approach	Mahdavi, H.	11:45
OP107	OA103	Quantum Conductance of Graphene Nanoribbon	Afshari, S.	12:00
OP108	OA105	Monitoring changes of Entropy and Specific heat capacity in Fullerenes	Esmaeilzadeh, S.	12:15
Second Session				
OP109	OA116	Density functional theory study of the adsorption of NO2 molecule on nitrogen-doped TiO2 anatase nanoparticles	Abbasi, M.	15:00
OP110	OA102	Rationalization of two-step mechanism of functionalization of single-walled carbon nanotubes with aryl diazonium salts: Comparison of OH and CH2CH3 substituent groups	Hoseinpour, S.	15:15
OP111	OA106	The Computaional Comparison of deformation effects on Structural and Electronical Properties of Carbon and Boron-Nitride Nanotubes	Fallah, A.	15:30
OP112	OA120	The study of interaction formaldehyde (HCHO) on surface of single- walled carbon nanotube (8, 0) by DFT calculation	Kazemi Babaheydari, A.	15:45
OP113	OA110	Investigation of aromaticity by using NICS-scan Index	Esmaeili, A.	16:00
OP114	OA113	DFT calculations on the cis and trans isomers of a nanosize organotin(IV) complex	Shariatinia, Z.	16:15
OP115	OA115	H2 and NO chemisorbtion on the surface of single-walled Nanotubes C-C by Density Function Theory (DFT)	Soleymanabadi, H.	16:30
OP116	OA111	DFT calculations on the structures of two novel nanosized phosphoric triamides	Shahidi, S.	16:45
OP117	OA121	Theoretical Investigations on Electronic Structure of Boron Nitride (BN) Fullerene-Like Structures: A Density Functional Theory Study	Fakhari, Z.	17:00

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New Code	Old Code	Title of Oral – Panel 2: Medicinal Computations	Presented by	Time
OP218	OA204	Theoretical Study of Conformation and Drug Delivery Mechanism of Doxorubicin-Conjugated Glycol Chitosan, via H bond (GC/DOX) Poly ethylene Glycol chain, by Hartree fock Method	Fattahi, A.	10:30
OP219	OA202	Theoretical study on nanoencapsulation and cytotoxic activity of titanocene with α-, β-, and γ-cyclodextrin	Karimi, F.	10:45
OP220	OA205	Theoretical Study of Conformation and Drug Delivery Mechanism of Doxorubicin- Conjugated Glycol Chitosan, Via Cis- Aconityl, By Hartree Fock Method	Daspak, T	11:00
OP221	OA206	DFT studies of transmission dopamine drug on the surface functionalized carbon nanotubes	Arjmand nezhad, N.	11:15
OP222	OA207	Theoretical Study on the Geometrical Properties of Paclitaxel Conjugated to Nanoparticle Chitosan Biopolymer Along with ethylene glycol chains	Akbarian, N.	11:30
OP223	OA208	Sidewall Covalently Functionalization of SingleWall Carbon Nanotubes for Drug Delivery Applications	Nasseh, S.	11:45
OP224	OA211	The effect of reaction between benzylidene benzohydrazide and Fullerene	Dehghan Tezerjani, A.	12:00
OP225	OA212	The Quantum Investigation of Polymeric Nanoparticles as Drug Carriers	Madadi Mahani, N.	12:15
Second Session				
OP226	OA213	The study of drug delivery dopamine by fictionalization on C60: by DFT calculation	Tavakoli, Kh.	15:00
OP227	OA215	DFT study of Mustard adsorption from head of sulfur on the Aluminum-Nitride nanotubes with different diameter	Bolbol Amiri, M.	15:15
OP228	OA216	The comparison of NMR tensors and NQR frequencies of hallucinogenic harmine compound in the gaseous phase	Ahmadinejad, N.	15:30
OP229	OA217	Interaction of different aminoacids with a biologic acid nanoparticle	Shajareh Tuba, R.	15:45
OP230	OA218	calculations of basis set effects on the NMR chemical shielding tensors data of amino acids in contact with nanotube	Kharghanian, L.	16:00
OP231	OA219	Computational investigation of structural properties for graphene functionalized azacytidine anticancer	Yaghoobi, R.	16:15
OP232	OA203	Determine how Nicotine Absorbed on the Surface of the Nanotubes using Density Function Theory (DFT)	Nouraliei, M.	16:30
OP233	OA201	The hydrogen bonding interactions among aspirin and organosilane nanoparticles	Nikfar, Z.	16:45
OP234	OA220	DFT Studies of Adsorption of Morphine molecule on BN and CC nanotubes	Golkish, B.	17:00

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New Code	Old Code	Title of Oral – Panel 3: Modeling & Simulations	Presented by	Time
OP335	OA310	Investigating Electron -Phonon Coupling in Carbon Nanotubes by Perturbation of the Hamiltonian	Moradi, P.	10:30
OP336	OA302	Co-doping effect on the hydrogen storage of single walled carbon nanotubes	Mohammadi, M.	10:45
OP337	OA308	Excitonic Effects and Optical Spectra of (8,0) Carbon Nanotube By Solving the Bethe-Salpeter Equation	Moradi, N.	11:00
OP338	OA305	Interaction of charged particles with nano wire with quantum model	Heidary, S.	11:15
OP339	OA306	Calculation of Current Density of GaAlAs Multi Quantum Barriers Under Electric Potential	Boodaghi Malidarre, R.	11:30
OP340	OA307	Propagation of electromagnetic wave in single-wall carbon nanotubes with different dielectric coefficient using a quantum hydrodynamic model	Soleimani, S.	11:45
OP341	OA309	Numerical Study of diameter effect on eletronic properties of single-walled BC3 nanotubes using tight-binding method	Farzadi, R.	12:00
OP342	OA311	The effect of nanoparticle size and refractive index on the surface plasmon resonance in three-particle array of ellipsoid gold nanoparticles	Taherkhani, R.	12:15
Second Session				
OP343	OA312	Nanoparticles in the medicinal industry based upon AHP method	Yaghoubi, Z.	15:00
OP344	OA313	QSPR modeling of stability constant of 18-crown-6 ethers derivatives with sodium cation	Hamzeali, H.	15:15
OP345	OA303	A Study on Thermodynamic Properties of Structure I CO2 Clathrate-Hydrate by Molecular Dynamics Simulation	Jamalzadeh, Z.	15:30
OP346	OA320	Investigation of effect of Carbon nanotube on solubility of different isomers of curcumin by Molecular Dynamic Simulation	Ighaei, M.	15:45
OP347	OA316	Molecular dynamics simulation of mechanical properties of carbon nanotubes (CNTs) and graphene sheets under mechanical loadings	Moradi, M.	16:00
OP348	OA317	Application of The Molecular Dynamics Simulations to Study The Cell Membrane	Vafaiee, M.	16:15
OP349	OA318	Analysis of adsorption kinetic of carbon molecular sieve synthesis process using molecular dynamics simulation	Yaghoubpoor, E.	16:30
OP350	OA319	Monte Carlo Investigation of Breast cancer protein(BRCA) and Effects of anticancer drugs of Gleevec and Tamoxifen using Computational methods	Rasoolzadeh, R.	16:45
OP351	OA304	Effect of Iridium nanoparticle size on the Iridium based on gamma-alumina catalyst: Using of molecular dynamics simulations	Salimi, M.	17:00

فهرست مقالات برای ارایه در قالب پوستر در کنفرانس نانو محاسباتی دانشگاه آزاد اسلامی واحد علوم دارویی ۲۷ بهمن ۱۳۹۱

۶- لطفاً New Code را برای مقاله خود به خاطر بسپارید، نصب پوسترها بر اساس New Code خواهد بود

۷- زمان نصب پوسترها در روز کنفرانس از ساعت ۱۳:۰۰ الی ۱۳:۳۰ خواهد بود، زمان ارایه پوسترهای نصب شده در روز کنفرانس از ساعت ۱۳:۳۰ الی ۱۵:۰۰ خواهد بود

۸- در تهیه پوستر به ابعاد مطلوب برای کنفرانس توجه فرمایید (ارتفاع: ۷۰ سانتی متر <> پهنا: ۵۰ سانتی متر)

۹- زبان مورد استفاده در تهیه پوستر دلخواه است

۱۰- در صورت نصب و ارایه پوستر گواهی ارایه مقاله صادر می شود

New Code	Old Code	Title of Poster	Presented by
PP001	x001	Investigation of strength of carbon nanotubes - silicon devices by lammps	Soleimani, Gh.
PP002	x002	Synthesis and Ab Initio Study of Nano Drug Carrier Based on Functionalized Single-Walled Carbon Nanotubes	Pakzadeh Masouleh, M.
PP003	x007	A survey upon Nano Barium nitride as a source of ammonia for the synthesis of highly substituted imidazoles	Motevalli, K.
PP004	x008-2	DFT Studies of NMR Parameters (NICS) for Nano Sheet B36N36 and C72	Soleymanabadi, H.
PP005	x009-2	Theoretical Computation of the Quantum Transport of Zigzag Mono-Layer Graphenes with Various z-Direction Width	Afshari, S.
PP006	x010	Polymer drug uptake: a molecular dynamics simulation study	Bahadorikhalili, S.
PP007	x014	Removal of detergents from hospital wastewater by using of nanofiltration in the membrane bioreactor (MBR)	Golbabaei Kootenaei, F.
PP008	x015	Copper Nitride thin films prepared by DC reactive magnetron sputtering and study the structural characteristics	Mahmoudi ghalvandi, M.
PP009	x017	rearrangement in unimolecular decomposition of FOX-7 Nitro- Nitrite	Sheikh, B.
PP010	x020	Optimal condition production current for glucose oxidase biosensor	Ramezani Azghandi, O.
PP011	x021-1	DFT Structural Analysis of the Complexes Composed Calix(4)arene Compound as Nano Chemisorbant of Hydrophilic α-Amino Acids	Nouraliei, M.
PP012	x021-2	Determination of the aromatic ring structure of C60 on using NICS analysis methods Oniom in theory Mp2	Nouraliei, M.
PP013	x022	Pre-concentration of Ascorbic Acid by SPME Method using Polypyrrole Nano-coating Combined with Advanced Chemometrics Method	Hoseini, S.S.

New Code	Old Code	Title of Poster	Presented by
PP014	x023	Fabrication of molecularly imprinted polymer coated carbon nanotubes modified electrode for detection of cholesterolcombined with advanced chemometrics method	Hemmati, Sh.
PP015	x025-1	DFT study of the Aluminum Nitride and Boron Nitride Nanocages	Vafaei, H.
PP016	x025-2	Theoretical study of nano-cage C18 and C24 and their comparison with boron nitride using DFT method	Vafaei, H.
PP017	x027-1	Synthesis of Nano Drug Carrier Based on Amino Functionalized MWCNTs	Zhalechin, M.
PP018	x027-2	Synthesis of New Derivatives of Functionalized Carbon Nanotubes and Comparison of Experimental Results with Theoretical Study on IR, RAMAN, and NMR spectroscopy	Zhalechin, M.
PP019	x028	Quantum Study of absorption of toxic gases in the air by the open nanocone coupled with the iron atom	Hadizadeh, M.H.
PP020	x030	Simple Quantitative Structure-Property Relationship modeling for prediction of the GC retention indices of essential oil compounds	Danandeh-Jenagharad, M.
PP021	x031-1	The study of electronic characteristics of di thiol stilbene Molecule, while applying bias	Hallaj Jahani, A.
PP022	x031-2	The Theoretical study of electron transport on Au- di thiol 3,3'- Bipyridyl -Au aromatic nanowire	Hallaj Jahani, A.
PP023	x034-1	Quantum calculations for the determination of molecular of compound 5-methyl-4-(1,3,5-triphenyl)-1H-1,2,4-triazole-4-yl-2H- 1,2,4-triazole-3(4H)-thione by methods of 1H NMR,13C- NMR spectroscopy and checking the results against empirical experiments	Boroushaki, T.
PP024	x034-2	The Usage comparison of occupancy parameters, gap of energy, ΔNmax at xylometazolin medicine ratio its medical conveyer nano	Boroushaki, T.
PP025	x034-3	Investigating structural properties for a triazolo 1,2,4-triazol derivative by DFT calculations	Boroushaki, T.
PP026	x035	Quantum computational of tautomerization on the structural properties of guanine nucleosbase	Sadeghi, S.S.
PP027	x036	Computational Study of Different Phases and Temperatures Effects on Single-Walled Carbon Nanotube and Herceptin Drug	Zare Karizaki, A.
PP028	x039	Molecular and Electric Properties of the Carbon Nanotube – Cyclophosphamide and Nanotube-Phosphoramide mustard New Compounds: density functional theory Studies	Kakaei, A.

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New Code	Old Code	Title of Poster	Presented by
PP029	x042	Modeling of interaction of polymer bundle and line defect in nematic liquid crystal	Ghorbani, M.
PP030	x046	Computational Studies on the Interaction between Serine and C20 fullerene, C19X (X=B, N) and metal encapsulated Na@C19X heterofullerene	Khalilzadegan, A.
PP031	x047-1	Applications of Nanotechnology in Papermaking Chemical Processes	Dashtbani, R.
PP032	x047-2	Producing Cellulose Nanofiber from Cotton Wastes by Electrospinning method	Dashtbani, R.
PP033	x048	Investigation of Ibuprofen adsorption on the single-walled carbon nanotube by Ab initio calculations method	Rakeb, A.
PP034	x049	Investigation of Diazepam adsorption on the single-walled carbon nanotube by Ab initio calculations method	Mohammadi, H.
PP035	x050	Ab initio studies of interactions between thioguanine and carbon / silicon graphene sheets	Karbalaei Mohammad, N.
PP036	x052	Investigation of Aspirin adsorption on the single-walled carbon nanotube by Ab initio calculations method	Doshmanziaria, S.
PP037	x054	The study rate of reaction increase electrophilicity in Allen using molecular orbital theory	Bahmani, Z.
PP038	x055	Investigation of Acetaminophen adsorption on the single-walled carbon nanotube by Ab initio calculations method	Ebrahimi, M.
PP039	x057	Controlled shapes and sizes gold nanoparticles production by biosynthesis	Shakoury hezejan, V.
PP040	x058	Natural convection heat transfer enhancement by nanofluids	Ershadi Farsani, H.
PP041	x059-1	Quantum Chemical Studies and NBO Analysis of (9,0) Zigzag & (5,5) Armchair Single Walled Carbon Nanotubes	Seyed Sadjadi, M.
PP042	x059-2	Determination of Chemical Properties of Small SWCNTs by Thermodynamic Investigation and NBO Analysis	Seyed Sadjadi, M.
PP043	x060	Theoretical Investigation & NBO Analysis on the Conductivity of Boron Nitride Nanotubes	Farhadyar, N.
PP044	x061	DFT Study, NBO Interpretation and HOMO-LUMO Analysis of (6,0) Zigzag Single Walled Carbon Nanotube	Azarakhshi, F.
PP045	x062	Comparison of Adsorption Capacity of C20, C19 Si and C19B fullerene clusters for H2 gas	Hasani, B.
PP046	x063	Computational Studies of New compounds Tacrine Alzheimer drug based on using Carbon Nanotube.	Mirali, M.
PP047	x065	Investigation of yield strain of hybrid nano composite with using Williamson- Hall equation and Hall- Petch effect	Baradaran Khaniani, M.
PP047	x065	Investigation of yield strain of hybrid nano composite with using Williamson- Hall equation and Hall- Petch effect	Rostamian, F.
PP048	x066	Synthesize of Polystyrene-zirconium dioxide hybrid nanocomposites	Abouk, Y.

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New Code	Old Code	Title of Poster	Presented by
PP049	x068	Modulus Modeling in Novel Photo-Crosslinkable Gelatin-clay Biohybrid Films	Bafkary, R.
PP050	x069-1	Theoretical investigation of Raman scattering for C60 in vacuum and benzene solutions	Karimi, F.
PP051	x069-2	nano-sized clusters of single cage to core–shell cage (Al2O3)n: Theoretical study	Karimi, F.
PP052	x072	Computational investigation of the optimum mechanism of Cox adsorption on the modified boron nitride nanotubes to develop the applications of gas sensors	Zahedi, H.
PP053	x076	Production of Nano Gold particles by six Streptomyces isolates of Kerman	Biglari, S.
PP054	x071	The interaction of Cytosine with Boron Nitride and Li-doped Boron Nitride Sheets: A DFT study	Kaeed, F.
PP055	x077-1	The Mathematical Modeling for Producing the Nanoparticles	yaghoubi, Z.
PP056	x077-3	Choosing a method for production of nanoparticles based on AHP technique	yaghoubi, Z.
PP057	x079-2	A comparative study of reaction between Chlorogenic acid and Fullerene	Dehghan Tezerjani, Ali
PP058	x080-1	Tautomerism in a novel phosphoramide nanoparticle	Shahidi, S.
PP059	x080-3	The cis and trans isomers of a new organotin(IV) nanoparticle	Shahidi, S.
PP060	x081-2	Calculation of transmission and longitudinal optical absorption of ellipsoidal silver nanoparticles by discrete dipole approximation	Taherkhani, R.
PP061	x082-2	Molecular structure of a new organosilane nanoparticle	Nikfar, Z.
PP062	x082-3	A novel organosilane nanoparticle prepared by condensation reaction	Nikfar, Z.
PP063	x075	Computational studies of absorbtion of Sox pollutant gases on the modified boron nitride graphene nano sheets	Karimi, E.
PP064	x083	Calculation of optical properties of spherical metal nanoparticles with core – shell structures	Sorayya, Sh
PP065	x084-2	Investigating Operation of undomped mode in Plasmon theire formation of Carbon Nanotubes	Moradi, P.
PP066	x085	Synthesis of new schiff bases using different derivatives of coumarin hydrazides as starting materials	Jafaritaba, M.S.
PP067	x086	Electronic properties of Zn1-xCrxS dilute magnetic semiconductor: first principle calculations	Boochani, A.
PP068	x087-2	Molecular mechanics study for adsorption of ammonia molecule onto rippled graphene sheet	Seyed Talebi, S. M.
PP069	x089-1	DesigneTargeted and controlled drug delivery system by anionic nanocomposite hydrogels	Alimardan, Z.

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New Code	Old Code	Title of Poster	Presented by
PP070	x089-2	DesigneTargeted and controlled drug delivery system by cationic nanocomposite hydrogels	Alimardan, Z.
PP071	x091-1	Optimization of the perovskite nano catalyst LaNiO3 to reduction of contaminators such as CO and NOx generated by the propellant gas generator combustion of fire extinguishing via value engineering and Taguchi experimental design method	Tahamtan, M.S.
PP072	x091-2	The comparison of micro and nano perovskite catalyst effect in reduction of contaminators such CO and NOx generated by the propellant gas generator combustion of fire extinguishing via Taguchi experimental design method	Tahamtan, M.S.
PP073	x092	Modeling of caffeine and its complex with Zn2+ and Investigation of spectral and thermodynamic properties, by calculational methods	Saneifar, H.
PP074	x096	Determination of Acidic Dissociation Constants of Xylenol Orange in Water Using Ab initio Methods	Ghadernezhad, F.
PP075	x073	Computational studies of NOX gaseous pollutants removal by their adsorption on the modified silicon carbide nanotubes	Iranimanesh, A.
PP076	x098	Interaction of NH_3, H_2 and CO molecules with SiC nanocluster surface	Zarorati, E.
PP077	x100	Antimicrobial properties of pineapple waste as drug precursors	Jafari, Z.
PP078	x101	Application of response surface methodology for optimization of the synthesis of Ti by sol-gel method	Damavandi, F.
PP079	x102	Solvent Effects on Acidic Dissociation Constants of Cytidine 5' Monophosphate Using Ab initio Methods	Halimi Jelodar, A.
PP080	x103	Investigation of cyclophosphamide drug attached armchair (4,4) carbon nanotube : Theoretical study	Razmand, M.
PP081	x105	Interaction between Amino Acids and Single-Walled Carbon Nanotube: A Theoretical Study	Tavousi, F.
PP082	x106	Molecular Dynamics Simulation of Nanoconfined Polymers	Rafi Dargahi, A.
PP083	x107	The study half metallicity of SrC/GaSb supercell; a density functional theory approach	Bashoki, Z.
PP084	x108	Determination of acidic dissociatoin constants of penicillamine in water using ab initio methods	Taherinasab, R.
PP085	x112-1	Structural study of the two isomers of a nanosized organotin(IV) complex	Shariatinia, Z.
PP086	x112-3	The most preferred coordination donor site of a phosphoric triamide nanoparticle	Shariatinia, Z.
PP087	x112-4	Chemical absorption of phosphoric triamide nanoparticles on the surface of a zigzag (10,0) carbon nanotube	Shariatinia, Z.
PP088	x112-5	NQR analysis of some phosphoric triamides grafted on the surface of a zigzag (10,0) carbon nanotube	Shariatinia, Z.
PP089	x113	Investigation of tautomerism and intramolecular hydrogen bond of 7-hydroxynaphthazarin	Yousofizadeh, M.

فهرست مقالات برای ارایه در قالب پوستر در **کنفرانس نانو محاسباتی** دانشگاه آزاد اسلامی واحد علوم دارویی ۲۷ بهمن ۱۳۹۱

New Code	Old Code	Title of Poster	Presented by
PP090	X115	Enhencing performance of pharmaceutical sensors by using Polyvinylpyrrolidone /Zink oxide hybrid nanocomposite	Derakhshi , M
PP091	x116	Multiwalled carbon nanotubes modified with 2-(2- hydroxy – 5- nitrophenyl) – 4.5 – diphenyl imidazole as efficient adsorbent (kinetic and thermodynamic investigation of Adsorption)	Jamshidi, M.
PP092	x120	Modifying a graphene layer by a thymine or a uracil nucleobase: DFT studies	Ravi, S.
PP093	x123	Structural properties investigation of Alumina nanoparticles biosensors	Salehi Moghadam, Z.
PP094	x125	MCR of the Quenching of the EEM of fluorescence of Aflatoxins (B1, G1) by Gold Nanoparticles	Saidi, A.
PP095	x130	Quantum study of absorption 1-methyl-2-thioxoimidazolin-4-one (T1)-iodine by single-walled carbon nanotube	Ghandchi, M.
PP096	x131	Simulation of interface of MnSe/CdSe in framework of density functional theory (DFT)	Saboori, S.
PP097	x132-1	Simulation	Khodabakhsh, S.
PP098	x132-2	Chemometrics	Khodabakhsh, S.
PP099	x132-3	Quantum computing	Khodabakhsh, S.
PP100	X136	Using Density Functional Theory calculations to optimize theoretical efficiency of Fullerenes-based Organic Solar Cells by substitution of hybrid elements	Javan Khosh Kholgh, M.
PP101	X138-2	Formation of some dipeptide nanoparticles between aminoacids and a biologic acid	Shajareh Tuba, R.
PP102	X138-3	A novel dipeptide formined by chitosan nanoparticles	Shajareh Tuba, R.
PP103	X140	siRNA transfection by Chitosan polysaccharide nanoparticle to inhibit influenza virus inhibition	Parvizi, Kh.
PP104	X143	Computational Studies of Electronic Properties for Pyridine Nanocompounds	Esmaili, E.
PP105	X145	Computational studies of thioguanine-nanocone hybrid	Beglari, M.
PP106	X146	Formation of chitosan nano chain and its properties: DFT studies	Malmir, M.
PP107	X147	DFT studies of structural properties for graphene-chitosan and graphene oxide-chitosan compounds and the effects of zidovudine on their properties	Mokhtari, A.
PP108	x149	Computational study of Ammonia adsorption on Boron Nitride fullerene – like structures	Mehdi Shishvan, S.

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New Code	Old Code	Title of Poster	Presented by
PP109	X150	QUANTUM MECHANICAL STUDY OF TRANSLATION ON CHEMICAL DRUGS USING CALIX[4]ARENE	Fathalizadeh, H.
PP110	x151	Drug Delivery Investigation on Bexarotene-Nanotube Complex In Cancer Treatment	Nouraldini, M.