BSW2011 Second Bozok Science Workshop: *Computational Chemical Physics,* Yozgat, April 21-23, 2011

Program

Time	Title
	21 April 2011, Thursday
10:00	Registration
10:30	Opening Remark
10:45	*Industrial applications of boron crystal* Ali OKATAN
	Lunch
13:30	*Melting process of nanocrystals by molecular dynamics simulations* Serap ŞENTÜRK DALGIÇ
14:00	*Functionalizing graphene by embedded boron clusters* Cem ÖZDOĞAN
14:20	*H(D) → D(H) + Cu(111) collision system: molecular dynamics study of surface temperature effects* Can Doğan VURDU
14:40	*Tuning the charge state of C_{60} nanoarrays by intercalation* Doğan ERBAHAR
15:00	Break
15:30	*Energetics of ion and ligand binding to GLTph and LeuT transporters* Murat ÇAVUŞ
15:50	*QSAR study between Inhibition efficiency and quantum chemical descriptor for some amino acids on cold rolled steel in HCl* Murat A. BAŞARAN
16:10	*Melting evaluation of Al-Pd nanoparticles by molecular dynamics simulations* Melek EKİNCEK
16:30	*DFT study of small clusters of Ti-B-N ternary systems* Nur ELMAS
16:50	***Poster Session***

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Time	Title
	22 April 2011, Friday
10:00	*Theoretical study on Zinc (II) and Ni (II) complexes of isatin and 5-methoxyisatin thiosemicarbazone derivatives* Fatma KANDEMİRLİ
10:30	*DFT investigation of planar and non-planar ScB_n (n=2-10) structures* Erdem Kamil YILDIRIM
10:50	*Electronic structure analysis of hydrogenated titanium doped cage boron clusters: DFT study of TiB_mH_n (n≤m, m=4–12 and n=1-12)* Muhammed AKAR
11:10	*Atom-yüzey etkileşmelerinde potansiyel enerji yüzeylerinin tanımlanması* Emrah KORKMAZ
11:30	*Pt-Au çekirdek-kabuk nanoparçacıkların moleküler dinamik simülasyonu yöntemi ile termodinamik özelliklerinin incelenmesi* Serkan KAYA
11:50	Lunch
13:30	Trip to Boğazkale (*Hattuşaş*)
	23 April 2011, Saturday
11:00	Trip to Sorgun (*Kaplıca*)

Posters

Time: 16:50 – 18:00

Title

Application of Gibbs free energy approach to calculate the melting behavior of Ag nanocrystals
Berna AKGENÇ

Synthesis and characterization of 3-hydroxy-n-(4-nitrophenyl) bezimidic acid
Yusuf AKKAYA

Synthesis and DFT study of some Cd(II) and Hg(II) complexes
Mecit AKSU

A DFT study on tautomerism and vibrational analysis of biomolecules: 3-deazauracil and 6-azauracil
Çağrı ÇIRAK

QSAR study of cytotoxicity effect on various cancer cells of some imidazo[1,2-α]pyrazine derivatives
Yadigar GÜLSEVEN SIDIR

Theoretical study on the inhibition effect of Azure A on mild steel in 1 M HCl
Demet ÖZKIR

Experimental and theoretical studies on the reactions 1,1'-(4-4'-(ethane-1,2-diyl)bis(4,1-phenylene)bis(azan-1-yl-1-ylidene)bis(methan-1-yl-1-ylidene)dinaphthalen-2-ol
Ali İhsan PEKACAR

Conformational stability, the spectroscopic (FT-IR and UV), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 6,8-diphenylimidazo[1,2-α]pyrazine molecule by ab initio HF and density functional methods
İsa SADIR

Theoretical study on some aminophosphine derivatives
Özlem SARIÖZ

Theoretical study on acidity-basicity behaviour of some substituted isatin thiosemicarbazone derivatives
Lokman ULUDAĞ

Molecular structure and vibrational Spectra of 2-, 3-, 4-ethylpyridine and 2-, 3-, 4-vinylpyridine by density functional theory and ab initio Hartree-Fock calculations
Yusuf SERT

Theoretical study on 4-(2-fluorophenyl)-1-(2-oxoindolin-3-ylidene) thiosemicarbazide
Yusuf AKKAYA

Calculation of electric capacitance by using extended Hubberd Model in nano-graphite ribbons
Osman ÖZSOY

Beş boyutlu Ising modelinde L=4 örgüsü için düzen parametresi ihtimaliyet dağılımı
Ziya MERDAN

Calix[4]arene bileşiğinin titreşim spektrumunun Yoğunluk Fonksiyonu Teorisiyle (DFT) incelenmesi
Alpaslan BAYRAKDAR

Quantum chemical computational studies on orto and meta-chlorobenzoic acid
Salih CINAKLI

DFT study of $C_{110}H_{80}$
Mustafa BÖYÜKATA