



Chemical Physics Congress IX

14-16 October 2010
Çeşme, İzmir/Türkiye



CPC-IX SCIENTIFIC PROGRAM

14.10.2010 (THURSDAY)

14.00-18.00 REGISTRATION

16.00-19.30 WELCOME COCKTAIL and A SOCIAL EVENT

15.10.2010 (FRIDAY)

		<u>ABSTRACT TITLE</u>	<u>CHAIR</u>
08.30	Opening Ceremony		
09.00-09.40	B. ERMAN (Invited Speaker)	Statistical Thermodynamics of Native Proteins and Drug Interactions	
09.40-10.00	Ş. SÜZER	Photovoltage and Photoconductivity as Probed by XPS	V. AVIYENTE
10.00-10.20	A.L. DEMİREL	Self-Assembly of Macromolecules Into Nanostructures in Solution	
10.20-10.40	S. CATAK	QM Metadynamics Study on Peptide Deamidation	
10.40-11.00	coffee break		
11.00-11.40	D. ALARA (Invited Speaker)	Effects of Molecular Structure on Electrical Response of Self-Assembled Monolayers - From Molecular Electronic Devices to Photoemission	
11.40-12.00	V. AVIYENTE	An Overview on Modeling The Free Radical Polymerization of Acrylate Derivatives	
12.00-12.20	M.F. DANIŞMAN	Structural and electronic investigation of organic thin films on Ag(111) and Au(111) surfaces	Ş. SÜZER
12.20-12.40	M.M. DEMİR	Towards transparent composites based on vinyl polymers and CeO ₂ nanoparticles	
12.40-14.00	lunch		
14.00-14.40	M. ERBUDAK (Invited Speaker)	Surface Faceting of the Icosahedral AlPdMn Quasicrystal	
14.40-15.00	E. SICILIA	VAM Synthesis Catalyzed by Bimetallic PdAu Surfaces. A Cluster Model Study of the Ensemble Effect Influence	
15.00-15.20	N.U. AYTEMİZ	Applications of Computer Simulation Techniques to Atmospheric Problems	T.YALÇIN
15.20-15.40	M. BİLSEL	Structural Properties of Peptides with Selective Binding Affinity for Carbon Nanotubes	
15.40-16.00	coffee break		
16.00-16.40	W. THIEL (Invited Speaker)	Theoretical Studies of Enzymatic Reactions	
16.40-17.00	A. TEKİN	Intermolecular potentials for Acetylene, Benzene and Acetylene – Benzene dimers and Acetylene – Benzene Aggregates	Z.ÇINAR
17.00-17.40	H.P. LUTHI (Invited Speaker)	Understanding Electron Delocalization and Conjugation Efficiency in Linearly pi-Conjugated Systems: From Complex Computations to Simple Concepts	
17.40-19.00	Poster I		



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16.10.2010 (SATURDAY)

ABSTRACT TITLE

CHAIR

09.00-09.40	I. BAHAR (Invited Speaker)	Functional Dynamics of Proteins Inferred from Structural Data and Elastic Network Models	
09.40-10.00	E. YURTSEVER	Structures and dynamics in ion traps	
10.00-10.20	E. ÖZKIRIMLI ÖLMEZ	Beta-Lactamase Ligand Binding: A Comparative Study	B.ERMAN
10.20-10.40	A.S. ÖZEN	A Multi-scale Computational Approach to the Self-Assembly of Fluorinated Block Copolymers	
10.40-11.00	coffee break		
11.00-11.40	H. ZIPSE (Invited Speaker)	Thermochemical Aspects of Radical Reactions	
11.40-12.00	T. BAŞTUĞ	Energetics of Ion and Substrate Binding to Glutamate Transporters	
12.00-12.20	N. ACAR	Interactions of Phenothiazine and Promazine with Some Pyrene Derivatives	E.YURTSEVER
12.20-12.40	E. EROĞLU	DFT-Based Qsar Study of Inhibition of Carbonic Anhydrase Isoforms (CAI, CAII and CAIX) by Sulfonamides	
12.40-14.00	lunch		
14.00-14.40	G. SCOLES (Invited Speaker)	Nanoscale Devices for Proteomics and Interactomics: Principles, Devices and Applications	
14.40-15.00	Z. ÇINAR	Origin of Visible-Light Activity of N-Doped TiO ₂ Photocatalysts	
15.00-15.20	E. YILDIRIM	Molecular Dynamics Study on the Interfacial Interactions in Polyethylene/Organoclay Nanocomposite Materials	N.U. AYTEMİZ
15.20-15.40	M. BÖYÜKATA	Metallo Boron Nano Structures: Their Hydrogen and Molecule Hosted Complexes	
15.40-16.00	coffee break		
16.00-16.40	N. RUSSO (Invited Speaker)	Computational Insight on Reactions catalyzed by metal containing enzymes	
16.40-17.00	E. ERDEM	Quantum size effects in functional ferroelectric nanomaterials	M.YURTSEVER
17.00-17.20	Closing Session		
17.20-19.00	Poster II		
20.00	GALA DINNER		

SOCIAL EVENT

17.10.2010 (SUNDAY)

***The detailed information will be announced**

Option 1:

**BOAT TOUR ÇEŞME
(Daily Tour)**

**10:00 Departure from Hotel
18:00 Departure to Hotel**



Option 2:

Ephesus, House of Virgin Mary, Şirince Village Tour (Daily Tour, Tour Price 80 TL)

10:00 Departure from Hotel

18:00 Departure to Hotel

(Entrance of Ephesus and House of Virgin Mary, guide service and lunch included in fee)

Ephesus



<http://www.selcuk.bel.tr/eng/selcuk.php?module=21>

House of Virgin Mary



<http://www.selcuk.bel.tr/eng/selcuk.php?module=9>

Şirince



<http://www.selcuk.bel.tr/eng/selcuk.php?module=62>



<http://www.selcuk.bel.tr/eng/selcuk.php?module=62>