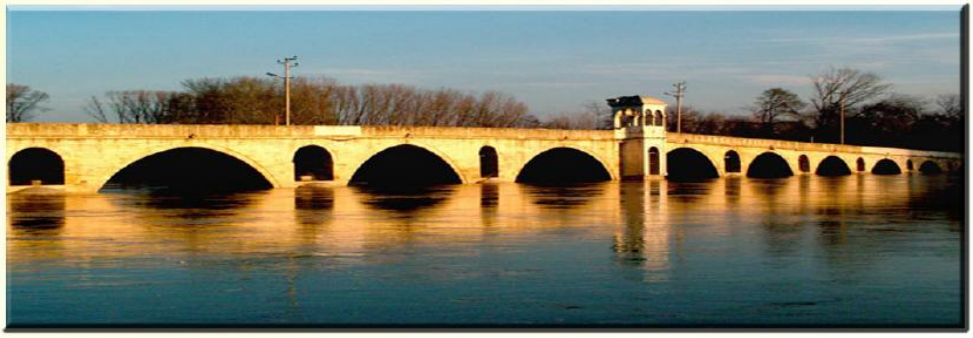
TRAKYA ÜNİVERSİTESİ

Sıvıhal Fiziği Çalışma Grubu

14. ULUSAL SIVIHAL FİZİĞİ SEMPOZYUMU

23-26 ARALIK 2010

Trakya Üniversitesi Balkan Kongre Merkezi, EDİRNE



KONUŞMA VE BİLDİRİ ÖZETLERİ

ABSTRACT BOOK

Destekleyen Kuruluşlar:

TÜBİTAK

SEMPOZYUM BİLİM KURULU

Prof. Dr. Zehra Akdeniz	*Piri Reis Üniversitesi*
Prof. Dr. Sevim Akyüz	*Kültür Üniversitesi*
Prof. Dr. A. Nihat Berker	*Sabancı Üniversitesi*
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Prof. Dr. Yani Skarlatos	*B*oğaziçi *Üniversitesi*
Prof. Dr. Bilal Tanatar	*Bilkent Üniversitesi*
Prof. Dr. Hasan Tatlıpınar	*Yıldız Teknik Üniversitesi*
Prof. Dr. Mehmet Tomak	*Ortadoğu Teknik Üniversitesi*
Prof. Dr. İskender Yılgör	*Koç Üniversitesi*
Prof. Dr. Ersin Yurtsever	*Koç Üniversitesi*

SEMPOZYUM DÜZENLEME KURULU

Prof. Dr. Zehra Akdeniz	*Piri Reis Üniversitesi*
Yrd. Doç.Dr. Zeynep Çiçek Önem	*İstanbul Üniversitesi*
Yrd. Doç.Dr. Ali Karaman	*İstanbul Üniversitesi*

SEMPOZYUM YEREL DÜZENLEME KURULU

Prof. Dr. Ş. Erol Okan	*Trakya Üniversitesi*
Yrd. Doç.Dr. Şaban Aktaş	*Trakya Üniversitesi*
Yrd. Doç. Dr. Figen Boz	*Trakya Üniversitesi*
Dr. A. İhsan Meşe	*Trakya Üniversitesi*

Sıvıhal Fiziği Çalışma Grubu

14. ULUSAL SIVIHAL FİZİĞİ SEMPOZYUMU

23-26 Aralık 2010

Trakya Üniversitesi, Balkan Kongre Merkezi, Edirne

PROGRAM

23 December/Aralık 2010, Thursday/Perşembe

10.00-13.30 Registration/Kayıt

13.30-14.00 Opening/Açılış

Chairperson/Oturum Başkanı: Zehra Akdeniz

14.00-14.40 *Frozen Impurity and Localized/Delocalized Electron Effects in Electronic Models: Renormalization-Group Theory*
A.Nihat Berker (Sabancı Üniversitesi)

14.40-15.20 *Ground state degeneracy of a strongly interacting Bose-Fermi mixture in a 1D harmonic confinement*
Patrizia Vignolo (Institut Non Linéaire de Nice, CNRS-France)

BREAK / ARA

Chairperson/Oturum Başkanı: Gülsen Tezgör

16.00-16.40 *Capillary electrophoretic methods for food toxins generated from natural foodingredients*
Bedia Erim Berker (İstanbul Teknik Üniversitesi)

16.40-17.20 *Vibrational Properties of Metal nanowires under Tensile Stress*
Sondan Durukanoğlu Feyiz (Sabancı Üniversitesi)

17.20-17.40 *Size Effect on Melting Process of ZnO Nanowires*
Serap Şentürk Dalgıç, Sedat Şengül (Trakya Üniversitesi)

17.40-18.00 *Sıvı fazdaki tuzlar için transport özellikleri*
Eren Tosyalı, Serpil Çıkıt , Zehra Akdeniz (İstanbul Üniversitesi)

18.00-20.00 COCTAIL/KOKTEYL

24 December/Aralık 2010, Friday/Cuma

Chairperson/Oturum Başkanı: Nurşen Seçkin Görgün

09.30-10.10 *Manipulating organizational pathways of biological molecules*
Ali Rana Atilgan, Ayse Ozlem Aykut, Deniz Turgut, and Canan Atilgan . (Sabancı Üniversitesi)

10.10-10.50 *Modified Surfaces with Tunable Interactions Shed Light on Water-Substrate Coupled Dynamics*
Canan Atılgan, Cem Servantie, Ali Rana Atılgan (Sabancı Üniversitesi)

BREAK / ARA

Chairperson/Oturum Başkanı: Fikret İşık

11.10-11.30 *Liquid Structure calculations of molecular TeF6*
Hülya Kes, Serap Şentürk Dalgıç (Trakya Üniversitesi)

11.30-11.50 *The effects of the laser and magnetic fields on the double quantum well*
Figen Karaca Boz, Şaban Aktaş, Ş.Erol Okan (Trakya Üniversitesi)

11.50-12.10 *Raman Spectra of molten MCl_3 Systems*
Batu Hunca, Şaban Aktaş, Ş.Erol Okan, Zehra Akdeniz (Trakya Üniversitesi)

12.10-14.00 LUNCH/ÖĞLE YEMEĞİ

Chairperson/Oturum Başkanı: Hülya Kes

14.00-14.40 *BCS-BEC Crassover in density imbalanced electron-hole bilayers*
Bilal Tanatar and A. Levent Subasi (Bilkent Üniversitesi)

14.40-15.00 *Size and shape Effects on Melting behaviors of Au nanocrystals by Molecular Dynamics Simulation*
Serap Şentürk Dalgıç, Ünal Dömekeli (Trakya Üniversitesi)

15.00-15.20 *Liquid -to-glass transition in bulk glass-forming $Cu_{50}Ti_{25}Zr_{25}$ alloy using molecular dynamics simulation*
Serap Şentürk Dalgıç, M.Celtek(Trakya Üniversitesi)

BREAK / ARA

Chairperson/Oturum Başkanı: Nimet Zaim

16.00-16.20 *Melting evolution of bimetallic TiAl nanoparticles*
Serap Şentürk Dalgıç, Melek Ekincek (Trakya Üniversitesi)

16.20-16.40 S*pontaneous Formation of A Nanotube From A Square Ag Nanowire*
Mine Konuk, S. Durukanoglu (İstanbul Teknik Üniversitesi)

16.40-17.00 *Embedded Atom Method Potentials for Al,Ni,Co Metals and Their Alloys*
Berk Onat, S. Durukanoğlu (İstanbul Teknik Üniversitesi)

BREAK / ARA

17.30-18.30 *Talent and Jealousy on Water: Admiral Alcibiades and his Oligarchical environment*
A.Nihat Berker (Sabancı Üniversitesi)

20.00- DINNER/ SEMPOZYUM YEMEĞİ

25 December/Aralık 2010, Saturday/Cumartesi

Chairperson/Oturum Başkanı: Abdullah Bilekkaya

09.30-10.10 *Phase Transitions in Red Seaweeds*
Önder Pekcan (Kadir Has Üniversitesi)

10.10-10.50 *DFT Study of Al_xB_y (x,y=1-4) Micronanoalloys and Their Hydrogenated Complexes*
M. Böyükata , Z. B. Güvenç (Bozok Üniversitesi)

BREAK / ARA

Chairperson/Oturum Başkanı: Sedat Şengül

11.10-11.50 *Investigation of Phase Transitions in Polar Liquid Crystals via Birefringence Measurements*
Mehmetcan Çetinkaya, Selen Erkan, Haluk Özbek, Sevtap Yıldız (İstanbul Teknik Üniversitesi)

11.50-12.30 *Geometric Correlations and Breakdown of Mesoscopic Universality in Spin Transport*
İnanç Adagideli (Sabancı Üniversitesi)

12.30-12.50 *Structural and Energetic Analysis of $Pt_6(CO)_m$ and $B_nPt_{6-n}(CO)_6$ (m,n≤6) clusters*
N. Özbey, M. Böyükata, Z. B. Güvenç (Bozok Üniversitesi)

26 December/Aralık 2010, Sunday/Pazar

11.00-16.00 *Çalıştay*

Frozen Impurity and Localized/Delocalized Electron Effects in Electronic Models: Renormalization-Group Theory

A.Nihat Berker

Sabancı Üniversitesi

Ground state degeneracy of a strongly interacting Bose-Fermi mixture in a 1D harmonic confinement

Patrizia Vignolo

Institut Non Linéaire de Nice, CNRS-France

We investigate the ground state degeneracy of a strongly interacting mixture of a Tonks-Girardeau (TG) gas (1D Bose gas with point hard cores) and of a non-interacting Fermi gas (1D spin-aligned Fermi gas) trapped in a harmonic confinement.Prescriptions are given to construct the basis of the degenerate manifold for the TG limit.

Capillary electrophoretic methods for food toxins generated from natural food ingredients

Bedia Erim Berker

İstanbul Teknik Üniversitesi

Vibrational Properties of Metal nanowires under Tensile Stress

Sondan Durukanoğlu Feyiz

Sabancı Üniversitesi

We have investigated the vibrational density of states (VDOS) of a thin Cu nanowire with $<100>$ axial orientation and considered the effect of axial strain. The VDOS are calculated using a real space Green's function approach with the force constant matrices extracted from interaction potential based on the embedded atom method. Results for the vibrational density of states of a strain-free nanowire show quite distinctive characteristics compared to that of a bulk atom, the most striking feature of which is the existence of high frequency modes above the top of the bulk spectrum. We further predict that the low frequency characteristics of the VDOS reveal the quasi-1 dimensional (Q1D) behavior only when the wire is extremely thin. Through decomposition of VDOS into local atoms we also exhibit that while the anomalous increase in low frequency density of states is mainly due to the corner atoms, the enhancement in high frequency modes is primarily moderated by core atoms. We, additionally, find that while the high frequency band above the top of the bulk phonon shifts to higher frequencies, the characteristics at low frequencies remains almost the same upon stretching the nanowire along the axial direction.

Size Effects on Melting Process of ZnO Nanowires

Serap ŞENTÜRK DALGIÇ and Sedat ŞENGÜL

Department of Physics, Faculty of Science, University of Trakya, 22030, Edirne-TURKEY

The shell model molecular dynamics (MD) simulations are carried out to investigate the melting process of zinc oxide nanowires with square cross-sections labelled as nanobelts. The interatomic interactions have been defined by the Coulomb, Van der Waals, and repulsion interactions. In this work, the wires of four diferent lateral dimensions have been studied They have been generated by assembling the rocksalt unit cell along [001] crystalline axes. Periodic boundry conditions have applied only along their length. The size effects on melting of nanowires has been investigated. The structural analysis of MD simulations of ZnO nanobelts are also presented and compared with available results. Some dynamic properties such as mean square displacement and diffusion coefficient have also calculated to get detailed information about the nature of melting process of ZnO nanobelts. Calculations show that melting temperatures of ZnO nanobelts are lower than that of bulk and higly related with the reciprocal of the dimensions of the nanowire.

*This work was supported by the Research Foundation of Trakya University under Project number TUBAP-2009/149

SIVI FAZDAKİ TUZLAR İÇİN TRANSPORT ÖZELLİKLERİ

Eren Tosyalı, Serpil Çıkıt , ve Zehra Akdeniz*

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Kriyolit (Na_3AlF_6) iyonik sıvısı için transport özellikleri moleküler dinamik simülasyonu[1] yardımıyla hesaplanmıştır. Polarizasyon etkilerini de içeren ve *ab initio* hesaplamaları ile kristal yapıda bulunan potansiyel parametrelerin oluşturduğu model [2], yapı hesaplamalarında kriyolitin kristal fazdaki moleküler dağılımını belirlemede başarılı sonuçlar vermiştir. Bu çalışmada kriyolit, ergime sıcaklığının üzerinde incelenerek bulunan yapısal fonksiyonlar yardımıyla sistemin başlıca moleküler birim yapısının yanısıra kriyolit kompozisyonundaki mevcut moleküllerin koordinasyon sayıları ve moleküler titreşim frekansları bulunarak literatürdeki deneysel ve teorik verilerle karşılaştırılmıştır. Ayrıca sistemin transport özellikleri olarak viskosite ve elektrik iletkenlik hesaplanıp literatürdeki deneysel değerleriyle kıyaslanmıştır.

[1] Z. Akdeniz, P. A. Madden J. Phys. Chem. B 110,6683-6691 (2006)
[2] Lindsay Foy and P. A. Madden J. Phys. Chem. B 110, 15302-15311 (2006)

Manipulating organizational pathways of biological molecules

Ali Rana Atilgan, Ayse Ozlem Aykut, Deniz Turgut, and Canan Atilgan

Sabanci University, School of Engineering and Natural Sciences, Tuzla 34956, Istanbul

Dynamics of biological molecules is adequately described herein by simple analytical methods. To efficiently monitor the equilibrium landscape and to orchestrate the allosteric pathway, we derive the following set of equations: i) the equilibrium equation of each repeating unit, ii) the constitutive relation for each (non)bonded short and/or long-range contact, and iii) the compatibility equation between the fluctuation of an element and fluctuations of its neighboring bonds. In this study, we demonstrate that cooperatively inserted intra-residue fluctuations, resembling different ligand interactions with the macromolecule, moderate the positional motion of the residues responsible for desired activities of the macromolecule. We identify a feedback mechanism between sensory regions and adaptively distributed actuating parts. We construct a template that is a subset of the native structure containing the controller and we show that the template is conserved within the families of evolved sequences. These templates are the key elements for protein-protein interactions. Domain motions of proteins, specifically, different binding partners of calmodulins and ferric binding proteins, are studied thoroughly as benchmarking cases. We study the relationships between the statistical and spectral properties of networks derived from these macromolecules so as to establish further form-function relationships.

Modified Surfaces with Tunable Interactions Shed Light on Water-Substrate Coupled Dynamics

Canan Atılgan, Cem Servantie, Ali Rana Atılgan

Sabanci University, Faculty of Engineering and Natural Sciences, Tuzla 34956, Istanbul

We tackle with the problem of how the dynamics along substrates are modified in the presence of water. For this purpose, we design model surfaces with different levels of wettability. This is achieved by altering the hydrophobicity and density of hydrocarbon segments grafted on graphene sheets. The main parameter monitored is the flexibility of the surface as a function of temperature, obtained from extensive molecular dynamics simulations. Three different factors contributing to the enhanced flexibility of the solvated substrate at higher temperatures are found, all depending on the different types of hydrogen bonding networks forming along the surface: (i) Local motions in the cage formed by neighboring tetrahedrally coordinated water hydrogen bonds are activated at ca. 180 K and lead to a change in the entropy, accompanied by the initial softening of the surface. These exist irrespective of the substrate type, therefore leading to a dynamical transition even for bare graphene immersed in water. (ii) Supplementary hydrogen-bonds are established in the presence of hydrophilic groups; their continuous extension into the bulk water provides additional flexibility to the surface, manifested as a broadening of the dynamical transition region. (iii) When the grafted groups have the right density to allow for formation of water pockets near the graphene surface, a third hydrogen bond network, in the presence of obstacles, form within the layer, leading to further flexibility at elevated temperatures. These ideas are supported by monitoring the diffusion of water along the surface and the coupling of water and surface relaxations.

Liquid Structure calculations of molecular TeF6

Hülya KES and Serap ŞENTÜRK DALGIÇ

Department of Physics, Trakya University, Edirne, 22030, Turkey

In the present study, the liquid structure of TeF6 clusters has been obtained with Variational Modified Hypernetted Chain (VMHNC) liquid state theory by assuming different forms for the interaction potential energy. Two different model potential for molecular interactions in clusters have been studied. First, pairwise-additive atom-atom intermolecular interactions based on Lennard-Jones potential functions proposed by Bartell were employed for the cluster. The potential of Proykova included a small coulomb term in the pairwise potential has been also calculated inorder to find the polarization effects on the structure. These potentials have used as input data for structure calculations. The configuration part of free energy of VMHNC has been computed as a function of temperature. The VMHNC static structure and pair correlation functions of molecular TeF6 cluster at different temperatures and near melting have been calculated and compared with available results.

The effects of the laser and magnetic fields on the double quantum well

Figen Karaca Boz, Şaban Aktaş, Şevket Erol Okan

Department of Physics, Trakya University, 22030 Edirne, Turkey

We have studied the effects of the laser and magnetic fields on the binding energy of the impurity in double square and parabolic quantum wells for various barrier potentials. The ground state energy has been calculated with finite different method under effective mass approximation. Within a variational scheme, the binding energy is obtained as a function of the laser dressing parameter for the different magnetic field values. The results show that the electronic properties strongly depend not only on the laser dressing parameter, but also on the applied magnetic field and the impurity position.

Raman Spectra of Molten MCl_3 Systems

Batu Hunca, Şaban Aktaş, Şevket Erol Okan, Zehra Akdeniz*

Department of Physics, Trakya University, 22030, Edirne, Turkey

**Piri Reis University, İstanbul, Turkey*

In this work we studied the structure and theoretical Raman spectras of the MX_3 systems. With the use of molecular dynamics program where an appropriate potential model is used, structure and theoretical Raman spectra calculations have been done in the liquid phase of the systems of interest.

*This work was supported by the Research Foundation of Trakya University under Project number TUBAP-2010/33

BCS-BEC CROSSOVER IN DENSITY IMBALANCED ELECTRON-HOLE BILAYERS

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Department of Physics, Istanbul Technical University, Maslak, Istanbul, Turkey

We study excitonic condensation in a semiconducting electron-hole bilayer system with unequal layer densities at zero temperature. Using mean-field theory we solve the BCS gap equations numerically and investigate the effects of intra- and inter-layer interactions.

We analyze the stability of the Sarma phase with $\mathbf{k},-\mathbf{k}$ pairing by calculating the superfluid mass density and also by checking the compressibility matrix. We find that with bare Coulomb interactions the superfluid density is always positive in the Sarma phase, due to a peculiar momentum structure of the gap function originating from the singular behavior of the Coulomb potential at zero momentum and the presence of a sharp Fermi surface. Introducing a simple model for screening, we find that the superfluid density becomes negative in some regions of the phase diagram, corresponding to an instability towards a Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) type superfluid phase.

Thus, intra-layer interaction and screening together can lead to a rich phase diagram in the BCS-BEC crossover regime in electron-hole bilayer systems.

Size and shape effects on melting behavior of Au nanocrystals by molecular Dynamics simulations

Serap ŞENTÜRK DALGIÇ and Ünal DÖMEKELİ

Department of Physics, Trakya University, 22030, Edirne, Turkey

Molecular Dynamics (MD) simulations were performed on series of gold nanocrystals (nanoparticles (Nps), nanowires (Nws) and nanoplates) comprised of different sizes, to study their structures and properties during heating. The melting process of gold nanocrystals is studied by MD simulations with the quantum Sutton–Chen many-body force field. The nature of melting of Au nanocrystals has been also discussed with the analysis of some thermodynamic properties deduced from MD simulations such as cohesive energy, heat of fusion and melting point. In order to understand the shape effects on melting point of Au nanocrystals, we have interested in 0D, 1D, 2D dimensions of nanocrystals. Thus, size-, dimensionality-, and shape dependent melting temperatures of Au nanocrystals have been determined. MD simulation results are also compared with available experimental data and other theoretical results.

Liquid -to-glass transition in bulk glass-forming $Cu_{50}Ti_{25}Zr_{25}$ alloy using molecular dynamics simulation

S SENTURK DALGIC[1] AND M.CELTEK[2]

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[2]University of Trakya, Educational Faculty, 22050 Edirne, TURKEY

We report results from molecular dynamics (MD) studies concerning the microscopic structure of the ternary, bulk metallic glass-forming $Cu_{50}Ti_{25}Zr_{25}$ alloy using the newly developed for the ternary Cu-Ti-Zr system [1]. An atomic description of the melting, glass formation and crystallization process has been analyzed using heating and different cooling rates. Understanding of the nature of Glass Forming Ability (GFA) of this alloy, GFA parameters, glass transition temperature (T-g), melting temperature (T-m), reduced glass transition temperature, the supercooled liquid region and other parameters were simulated and compared with experiments. The computed Glass Forming Ability (GFA) parameters are in good agreement with experimental data. The structure analysis of the $Cu_{50}Ti_{25}Zr_{25}$ based on molecular dynamics simulation will be also presented and compared with available MD results [2]. We have also discussed the crystallization transition with two different interatomic potentials used in this work. The computed structure and thermodynamics properties will be also presented.

[1] S. Senturk Dalgıç and M. Çeltek (unpublished results).

[2] S. Senturk Dalgıç and M. Çeltek, "MD study of the ternary $Cu_{50}Ti_{25}Zr_{25}$ BGF alloy, Proccedings of Liquid and Amorphous Metals Conference-LAM14, Rome-Italy , 2010 (in press)

Melting evolution of bimetallic TiAl nanoparticles

Serap ŞENTÜRK DALGIÇ and Melek EKİNCEK

Department of Physics, Trakya University, Edirne, 22030, Turkey

In the present study, the melting process of spherical TiAl binary nanoparticles with the diameters around 3–9nm has been investigated by theoretical models. Size dependent melting temperature of spherical shaped nanoparticles with free standing has obtained from the thermodynamic models. The liquid drop model for binary nanoparticles has been developed in this work from the study of Nanda . We have also presented a new model for the size effect on melting temperature of nanoparticles deduced from the modelled by Lu and co-workers. Size depending melting properties of TiAl nanoparticles are investigated with the composition of $Ti_{50}Al_{50}$. The obtained results reveal that the melting temperatures of nanoparticles are inversely proportional to the reciprocal of the nanoparticle size, and are in good agreement with the Molecular Dynamics (MD) predictions [1].

[1] S. Senturk Dalgıç (unpublished results).

Spontaneous Formation of A Nanotube From A Square Ag Nanowire

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[2] *Faculty of Engineering and Natural Sciences, Sabancı University, 34956 Istanbul, Turkey*

The recently observed phenomenon of spontaneous formation of a tube from a regular, square Ag nanowire [1] has been investigated through molecular static and dynamic simulations based on the interaction potentials obtained from the embedded atom method [2]. With molecular static calculations, we investigate the effect of strain on this particular type of transformation by focusing specifically on square Ag nanowires. With molecular dynamic simulations, on the other hand, we discuss the effect of temperature on the evolution of various lengths of silver nanowires during the elongation. Our results demonstrate that the formation of hollow structures is governed by the length of the nanowire and the applied gradient stress. Through ab initio calculations, we will also discuss on the electronic nature of this specific type of transformation.

This work is supported by TUBITAK under Grant No. 109T105.

[1] Lagos M.J., Sato, F., Bettini, J., Rodrigues, V., Galvao, D.S., Ugarte, D., Nature Nanotechnology, **4**, 149, (2009).

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Embedded Atom Method Potentials for Al, Ni, Co Metals and Their Alloys

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[2] *Faculty of Engineering and Natural Sciences, Sabancı University, 34956, İstanbul, Turkey*

We have developed semi-empirical and many-body type model potentials for Al, Ni, and Co metals to investigate the static and dynamic properties of their binary and ternary intermetallic compounds. The formalism is based on the embedded atom method, which basically involves a correct representation of pair interactions, atomic charge densities, and embedding energies in the functional form of charge densities. The key properties and fitting parameters for fitting procedure are carefully determined so that the potentials correctly model the properties of the respective metals and their alloys. We will compare our results with the available outcomes of experiments and first principle calculations.

[1] Daw M.S. and Baskes M.I., Phys. Rev. Lett., **50**, 1285 (1983)

[2] Daw M.S. and Baskes M.I., Phys. Rev. B, **29**, 6443, (1984)

[3] Foiles S. M., Baskes M. I., and Daw M. S., Phys. Rev. B, **33 7983**, (1986)

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Talent and Jealousy on Water: Admiral Alcibiades and his Oligarchical Environment

Nihat Berker

Sabancı Üniversitesi

Phase Transitions in Red Seaweeds

Önder Pekcan

Kadir Has Üniversitesi

In this work, the photon transmission technique was used to study phase transitions of red seaweeds (kappa carrageenan) in various salt solutions. Upon cooling gels performed coil to double helix (c-h) transitions however, upon heating gels presented double helix to coil (h-c) transitions by showing hysteresis type of transition paths. The transmitted photon intensity, Itr was monitored against temperature to study phase transitions. Transition temperatures were determined from the derivative of the transition paths. The critical gel fraction exponent β was measured and found to be around 1.00, in accord with the classical Flory-Stockmayer model. Photon transmission experiments for these gels were performed using an UV–visible (UVV) spectrometer for studying the swelling processes. Transmitted light intensity, Itr from the gel increased exponentially, when the carrageenan gels are immersed in water, as the swelling time increased. Increase in Itr was attributed to the disappearing of the lattice heterogeneities which might be originated between "frozen blob clusters" and holes in the swelling gel. Increase in Itr was modeled using the Li–Tanaka equation, from which the collective diffusion coefficients, Do were determined for various carrageenan content gels. It was observed that the Do values decreased as the carrageenan content was increased. In other words, gel segments move faster, when the gel swells in pure water and has less carrageenan content. Inclusion of salt ions into the swelling gel slows down the motion of gel segments presenting the lower Do values.

DFT Study of Al_xB_y (x,y=1-4) Micronanoalloys and Their Hydrogenated Complexes

M. Böyükata[1] and Z. B. Güvenç[2]

[1] Department of Physics, Bozok University, 66100 Yozgat, Turkey

[2] Department of Elect. and Comm. Eng., Çankaya University, 06530 Ankara, Turkey

We have been working on boron clusters and boron related nanostructures [1-4]. In this study, some parts of our findings related with B-Al nanoalloys and their hydrogenated complexes will be presented. The geometry optimizations have been carried out for Al_xB_y (x,y=1-4) and $Al_xB_yH_z$ clusters by employing Density Functional Theory (DFT), with B3LYP functional and 6-311++G(d,p) basis set [5]. Number of hydrogen atoms has been increased up to z=8 for Al_1B_1 and z=16 for Al_4B_4. For the other Al_xB_y nanoalloys the number of H atoms varies between these values. Their frequencies, electronic states, structural parameters and point groups have been determined. Their energetics with respect to their total energies, binding energies and HOMO-LUMO energy gaps have been analyzed as functions of the number of aluminum, boron and hydrogen atoms. In the energetically lower-lying stable structures of Al_xB_y clusters the boron atoms come closer to each other rather than to Al atoms. In the hydrogenated complexes mainly stable isomers have hydrogen atoms around the boron atoms.

Acknowledgment: This work is supported by TUBITAK (Grant No. 108T466).

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INVESTIGATION OF PHASE TRANSITIONS IN POLAR LIQUID CRYSTALS VIA BIREFRINGENCE MEASUREMENTS

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In this work we present new high temperature resolution data on the temperature dependence of the birefringence in the isotropic (I), nematic (N), smectic A (Sm A) phases of the polar liquid crystalline compound octylcyanobiphenyl $(8CB)$. From the analysis of the data, using the Vuks model for the internal electric field, we derived the information on the temperature behavior of orientational order parameter of $S(T)$. From a fitting procedure consisted with mean-field theory and the first order character of the N-I transition, we obtained a value of 0.236 ± 0.009 for the critical exponent β which describes the critical behavior of $S(T)$ near the N-I transition. The value obtained is in good agreement with the tricritical value $\beta = 0.25$ within the experimental resolution [1-3], and the values also found previously by refractive index data [4], dielectric constant anisotropy [5,6]. More recently, Lelidis [7], reported that coming from the isotropic phase a discontinuity of $S(T)$ was observed at the N-Sm A transition temperature (T_{NA}) in $8CB$ via birefringence measurements. Thus Lelidis concluded that the N-Sm A transition is driven first order by the nematic director thermal fluctuations which couple with the smectic order parameter. Lelidis [7] also observed that applying a strong enough electric field, the N-Sm A transition shifts to second order revealing the existence of a tricritical point. On the other hand, by inspection of the figure 2 in [7], it is questionable to conclude that the N-Sm A transition in $8CB$ is of first order since the temperature resolution in the vicinty of the transition is poor. In this work, we address the question whether, in the vicinity of T_{NA}, birefringence shows discontinuity in $8CB$ liquid crystal. Therefore we measured the temperature dependence of birefringence, near T_{NA} for $8CB$, with small scanning rates and high resolution (typical scan rate $9.2\ mK/min$). We observed, contrary to the assertion given in [7], no discontinous behavior in the birefringence at T_{NA} in $8CB$ liquid crystal. Additionally, in a temperature range of about $5.8\ K$ above and below T_{NA} pre-transitional evidence for the coupling between the nematic and smectic order parameters was observed. We show that the temperature derivative of the $S(T)$ curve below and above T_{NA} has the same power law behavior as the specific heat capacity with an effective critical exponent of 0.306 ± 0.027 [8]. Similar behavior of the temperature derivative of the $S(T)$ near T_{NA} for a non-polar liquid crystal compound 4-butyloxyphenyl 4'-decyloxybenzoate $(\overline{10}O\overline{4})$ was also reported previously by our group [9].

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Kuantum esevreli elektron akiskanlarinda geometrik korrelasyonlar ve mezoskopik evrenselligin spin tasiniminda kirilmasi

Geometric Correlations and Breakdown of Mesoscopic Universality in Spin Transport

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We construct a unified semiclassical theory of charge and spin transport in chaotic ballistic and disordered diffusive mesoscopic systems with spin-orbit interaction. Neglecting dynamic effects of spin-orbit interaction, we reproduce the random matrix theory results that the spin conductance fluctuates universally around zero average. Incorporating these effects into the theory, we show that geometric correlations generate finite average spin conductances, but that they do not affect the charge conductance to leading order. The theory, which is confirmed by numerical transport calculations, allows us to investigate the entire range from the weak to the previously unexplored strong spin-orbit regime, where the spin rotation time is shorter than the momentum relaxation time.

Adagideli et al., Phys. Rev. Lett. 105, 246807 (2010)

Structural and Energetic Analysis of $Pt_6(CO)_m$ and $B_nPt_{6-n}(CO)_6$ (m,n≤6) clusters

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In this preliminary work, structural and energetic analyses of carbon monoxide poisoned platinum microclusters are studied. CO molecules have been adsorbed onto octahedral Pt_6 cluster. Additionally, boron doped compositions have been investigated. Geometries of $Pt_6(CO)_m$ and $B_nPt_{6-n}(CO)_6$ (for m,n≤6) complexes have been systematically optimized by using Gaussian 03 [1]. Density Functional Theory (DFT) with B3LYP/CEP-121G has been used to perform all calculations. Structural stability, bond lengths, bond angles, total atomic charges, binding energies, binding energies per atom, HOMO and LUMO energies are the main interested physical quantities. This particular work will be a starting point for our progressive researches on influence of CO poisoning on metalloboron clusters and their hydrates, via following previous findings in the literature [2].

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