



**Sıvihal Fizîği Çalışma Grubu**  
**11. ULUSAL SIVIHAL FİZİĞİ SEMPOZYUMU**  
**27-30 EYLÜL 2007**  
**İstanbul Üniversitesi Baltalimanı Tesisleri, İstanbul**



**KONUŞMA VE BİLDİRİ ÖZETLERİ**  
**ABSTRACT BOOK**

**DESTEKLEYEN KURULUŞLAR: İSTANBUL ÜNİVERSİTESİ**  
**TÜBİTAK**

## SEMPOZYUM BİLİM KURULU

Prof. Dr. Zehra AKDENİZ	<i>İstanbul Üniversitesi</i>
Prof. Dr. Sevim AKYÜZ	<i>İstanbul Üniversitesi</i>
Prof. Dr. A. Nihat BERKER	<i>Koç Üniversitesi</i>
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Prof. Dr. Ersin YURTSEVER	<i>Koç Üniversitesi</i>

## SEMPOZYUM DÜZENLEME KURULU

Prof. Dr. Zehra AKDENİZ	<i>İstanbul Üniversitesi</i>
Prof. Dr. Handan GÜRBÜZ	<i>Yıldız Teknik Üniversitesi</i>
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*Sıvıhal Fiziği Çalışma Grubu*  
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**PROGRAM**

**27 September/Eylül 2007, Thursday/Perşembe**

- 14.00 – 17.00**     *Registration/Kayıt*
- 17.00 – 17.30**     **Opening/Açılış**
- 17.30 – 18.10**     *Static Structure Factor of Glasses and Jammed Materials at Low Temperatures*  
**Moises Silbert**  
**(IFRN, İngiltere)**
- 18.10 – 18.50**     *Probing Coupled Time Scales and Landscape Shifts in Functional Proteins*  
**Ali Rana Atılğan, Canan Atılğan**  
**(Sabancı Üniversitesi)**
- 18.50 – 19.30**     *Structure of Trivalent-Metal Halides from Simulations based on Intramolecular Force Laws*  
**Romina Ruberto**  
**(INFN, İtalya)**

**28 September/Eylül 2007, Friday/Cuma**

- 10.00 – 12.00**     *Working Grups Meetings I /Çalışma Grupları Toplantıları I*
- 12.30 – 14.00**     **LUNCH BREAK**
- 14.00 – 16.30**     *Working Grups Meetings II /Çalışma Grupları Toplantıları II*
- 16.30 – 17.00**     **BREAK/ARA**
- 17.00 – 17.40**     *Nonaqueous Capillary Electrophoresis for the Analysis of Acrylamide in Food*  
**Selda Başkan, F. Bedia Erim**  
**(İstanbul Teknik Üniversitesi)**
- 17.40 – 18.20**     *Self-Organization of Polymers in Liquid Media*  
**A. Levent Demirel**  
**(Koç Üniversitesi)**

- 18.20 – 19.00** *Unusual Phase Transitions in Complex Networks*  
**Michael Hinczewski**  
(Feza Gürsey Enstitüsü)
- 19.00 – 19.40** *Phycicochemical Features of Lanthanide-Alkali Metal Systems*  
**M. Gaune-Escard, L. Rycerz, E. Ingier-Stocka, S. Gadzuric**  
(IUSTI CNRS, Fransa)

**29 September/Eylül 2007, Saturday/Cumartesi**

- 10.30 – 11.00** *Temperature Dependence of the Tensile Properties of Carbon Nanotubes*  
**Gülây Dereli, Banu Süngü**  
(Yıldız Teknik Üniversitesi)
- 11.00 – 11.30** *Temperature Dependence of the Energy Band Gaps of Carbon Nanotubes*  
**Gülây Dereli, Necati Vardar, Önder Eyecioğlu**  
(Yıldız Teknik Üniversitesi)

**BREAK / ARA**

- 11.45 – 12.15** *Variable Morphologies of Styrene-co-perfloroalkylethylacrylate Co-oligomers in Different Concentrations of THF*  
**Gökhan Kaçar, Alimet Sema Özen, Canan Atılgan**  
(Sabancı Üniversitesi)
- 12.15 – 12.55** *Bhatia-Thornton Formalism for Multicomponent Mixtures*  
**Moises Silbert**  
(IFRN, İngiltere)
- 13.00 – 14.00** **LUNCH BREAK**
- 14.00 – 14.30** *Bir-Boyutlu Schrödinger Denkleminin Geniş Bir Çözümler Kümesi*  
**Bekir Karaoğlu**  
(Haliç Üniversitesi)
- 14.30 – 14.50** *Determination of Alginate Copolymer in Pharmaceutical Formulations by Micellar Electrokinetic Chromatography*  
**Nevin Öztekin, Selda Başkan, F. Bedia Erim**  
(İstanbul Teknik Üniversitesi)
- 14.50 – 15.10** *Alginat-Polietilenimin-Kil Nanokompozitlerinin Eldesi ve Fiziksel Özelliklerinin İncelenmesi*  
**F. Tezcan, E. Günister, F. Bedia Erim, N. Güngör**  
(İstanbul Teknik Üniversitesi)

**BREAK / ARA**

- 15.30 – 15.50** *Alternative Proton Conducting Membranes for High Temperature Fuel Cells*  
**Unal Sen, Nilay Unutulmaz, Ali Ata, Ayhan Bozkurt**  
**(Gebze Yüksek Teknoloji Enstitüsü)**
- 15.50 – 16.10** *An Experimental and Theoretical IR, Raman and X-Ray Study of 2-[(5-methylisoxazol-3-yl)amino]-2-oxo-ethyl methacrylate*  
**M. Karabacak, E. Şahin, M. Çınar, İ. Erol, M. Kurt**  
**(Kocatepe Üniversitesi)**
- 16.10 – 16.30** *Ground State Energy and Wigner Crystallization in Two-Dimensional Boson System*  
**A. İ. Meşe, P. Capuzzi, Z. Akdeniz, S. E. Okan, M. P. Tosi**  
**(Trakya Üniversitesi)**
- BREAK / ARA**
- 16.50 – 17.10** *The Role of Confinement and Shape on the Binding Energy of an Electron in a Quantum Dot*  
**S. Sucu, A. İ. Meşe, S. E. Okan**  
**(Trakya Üniversitesi)**
- 17.10 – 17.30** *The Electron Velocity in Incompressible Strips in Quantum Hall Bars*  
**D. Eksi, A. Siddiki, S. Aktaş, S. E. Okan**  
**(Trakya Üniversitesi)**
- 17.30 – 17.50** *Electric Field Effect on the Binding Energy of a Hydrogenic Donor Impurity in Quantum Well Wires of Different Shapes*  
**A. Bilekkaya, S. Aktaş, S. E. Okan**  
**(Trakya Üniversitesi)**
- 17.50 – 18.10** *Structure and Stability of Molecular Clusters in Pentafluoride Compounds and Polymerization in Their Vapour Phase*  
**Z. Çiçek Önem, Z. Akdeniz, M. P. Tosi**  
**(İstanbul Üniversitesi)**

**30 September/Eylül 2007, Sunday/Pazar**

- 10.00 - 12.00** *Working Grups Meetings III /Çalışma Grupları Toplantıları III*
- 12.30 - 14.00** **LUNCH BREAK**
- 14.30-** **EXCURSION / GEZİ**

# Probing Coupled Time Scales and Landscape Shifts in Functional Proteins

Ali Rana Atilgan and Canan Atilgan

*Faculty of Engineering and Natural Sciences, Sabanci University, 34956 Istanbul, Turkey*

We study the dynamics of folded proteins using all-atom and coarse-grained approaches. Our main goal is to understand how functionality is achieved once the protein folds into its three-dimensional structure. In all-atom models, we carry out classical molecular dynamics simulations in water and glycerol at a variety of temperatures, where the protein maintains its structure, but not necessarily its function (1,2). We explain the observed relaxation phenomena based on a viscoelastic model, asserting that the protein needs to form concerted interactions with a vicinal layer of solvent (3). To understand allosteric interactions in which a local change in one part of the protein induces other structural changes in distal parts, we study coarse grained models whereby the protein is considered as a network of its amino acids with links between residues in close proximity (4). We find that “information” is relayed in the protein through specially optimized pathways. The same principles apply for the commonly utilized interface residues in ligand-receptor interactions. The findings are corroborated by strong evolutionary conservation of key residues along these paths both within single proteins and in interacting ones (5). Moreover, using coarse-grained models, one may also reproduce residue-by-residue structural changes as determined from the X-ray structures of the ligand-free and ligand-bound forms. The latter is achieved by introducing small perturbations in specific residues, and calculating the changes in the coordinates through linear response theory (6-8). These changes are reversible, unless a small ligand that stabilizes certain preferred conformations is also present in the model. The latter observations are explained by shifts in the energy landscapes that are induced by forces, and cannot be accounted by modifications in temperature or solvent type.

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3. Atilgan, C., A. O. Aykut, and A. R. Atilgan. 2007. How a Vicinal Layer of Solvent Modulates the Dynamics of Proteins. *Biophys. J.* To appear.
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5. Atilgan, A. R., D. Turgut, and C. Atilgan. 2007. Screened non-bonded interactions in native proteins manipulate optimal paths for robust residue communication. *Biophys. J.* 92:3052-3062.
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7. Baysal, C. and A. R. Atilgan. 2001. Coordination Topology and Stability for the Native and Binding Conformers of Chymotrypsin Inhibitor 2. *Proteins* 45:62-70.
8. Ikeguchi, M., J. Ueno, M. Sato, and A. Kidera. 2005. Protein Structural Change Upon Ligand Binding: Linear Response Theory. *Phys. Rev. Lett.* 94:078102.

# **Determination of Alginate Copolymer in Pharmaceutical Formulations by Micellar Electrokinetic Chromatography**

**Nevin Öztekin, Selda Başkan and F. Bedia Erim**

*Department of Chemistry, Istanbul Technical University, Maslak 34469, Istanbul, Turkey*

A micellar electrokinetic chromatography method was developed for the separation and quantification of sodium alginate. The alginate peak migrated in the very short time of 1.33 min and calibrated easily though the polydisperse properties of alginates. The minimum detection limit (LOD) of the method was calculated as 0.393 mg/ml. This analysis method was successfully applied to the alginate quantification in an antacid pharmaceutical formulation. With liquid formulations injected directly without any pre-separation process, precise and reproducible analysis results were obtained.

# Electric Field Effect on the Binding Energy of a Hydrogenic Donor Impurity in Quantum Well Wires of Different Shapes

**A. Bilekkaya<sup>a</sup>, S. Aktaş<sup>b</sup>, S. E. Okan<sup>c</sup>**

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In this work, we present a study of the role of the electric field on the binding energy of a hydrogenic donor impurity in GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As quantum well-wires (QWWs) of different shapes using the finite difference method. It is shown that the method is able to calculate all energy states for any given QWW shape in the presence of an applied electric field. Then, the binding energy of a hydrogenic impurity is found employing a variational method. Our results indicate that the impurity binding energy depends strongly on the structural confinement and also, on the applied electric field.

**Key words:** binding energy, quantum well-wire, finite difference, different shape.

# **An Experimental and Theoretical IR, Raman and X-Ray Study of 2-[(5-methylisoxazol-3-yl)amino]-2-oxo-ethyl methacrylate**

**M. Karabacak<sup>a</sup>, E. Sahin<sup>b</sup>, M. Cinar<sup>a</sup>, İ. Erol<sup>c</sup> and M. Kurt<sup>d</sup>**

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Molecular structure of the methacrylate monomer, 2-[(5-methylisoxazol-3-yl)amino]-2-oxo-ethyl methacrylate (IAOEMA) was determined by X-ray diffraction analysis. Furthermore, the Fourier Transform Raman and Fourier Transform Infrared spectra of IAOEMA were recorded in the solid phase. The equilibrium geometry, harmonic vibrational frequencies, infrared intensities and Raman scattering activities were calculated by Hartree-Fock (HF) and density functional (B3LYP and B3PW91) methods with the 6-31G(d, p) and 6-311G(d, p) basis sets. The vibrational frequencies were calculated and scaled values have been compared with experimental FT-IR and FT-Raman spectra. The scaled theoretical wavenumbers showed very good agreement with the experimental values. The optimized bond lengths and bond angles show the best agreement with the experimental results.

# **Self-Organization of Polymers in Liquid Media**

**A. Levent Demirel**

*Koc University, Chemistry Department, Sariyer 34450, Istanbul, Turkey*

Polymeric molecules self-organize in liquids into various structures mainly due to selective interactions of liquid molecules with certain parts of the polymer molecules. After a brief introduction of the fundamentals of self-organization, I will focus on structure formation of poly(2-alkyl-2-oxazoline)s in aqueous solution. Poly(2-alkyl-2-oxazoline)s represent an important class of tertiary polyamides whose properties can be adjusted from amorphous to crystalline and from hydrophilic to hydrophobic depending on the nature of the side chain. Poly(2-isopropyl-2-oxazoline) (PIPOX) is the only polymer in this class which is both crystalline and soluble in water. PIPOX self-organizes into crystalline nanofibers in aqueous solution above lower critical solution temperature. By scanning force microscopy, differential scanning calorimetry and X-ray diffraction measurements, these nanofibers are shown to be produced through a slow directional crystallization process. A structural model of the crystal that reproduces the experimental data will be presented. Based on the experimental and modelling results, the role of hydrophobic interactions, dipolar interactions and backbone solvation in possible structure formation mechanisms will be discussed.

# The Electron Velocity in Incompressible Strips in Quantum Hall Bars

**D. Eksi<sup>a</sup>, A. Siddiki<sup>b</sup>, S. Aktas<sup>a</sup>, S. E. Okan<sup>c</sup>**

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We report on our theoretical investigation of the effects of the confining potential profile and sample size on the electron velocity distribution in (narrow) quantum Hall systems. The electrostatic properties of the electron system are obtained by the Thomas-Fermi-Poisson non-linear screening theory. The electron velocity distribution as a function of the lateral coordinate is obtained from the slope of the screened potential at the Fermi level and within the incompressible strips. Our findings are in good agreement with the recent experiments.

# **Nonaqueous Capillary Electrophoresis for the Analysis of Acrylamide in Food**

**Selda Başkan and F. Bedia Erim**

*Department of Chemistry, Istanbul Technical University, 34469 Maslak, Istanbul, Turkey*

A nonaqueous capillary electrophoresis method was developed for the quantitative determination of acrylamide in processed food. The method is premised on the modification of the aqueous acid-base character of acrylamide in an organic solution. Acrylamide, which is a polar molecule in aqueous solution, in a low pH environment in acetonitrile acquires a proton and thereby migrates under its own electrophoretic mobility in capillary electrophoresis. Thus, nonaqueous separation of acrylamide was achieved employing 30 mmol/l HClO<sub>4</sub> in acetonitrile as the running electrolyte. The detection limit of the method for acrylamide was found as 0.041 µg/ml using UV detection at 200 nm. The run-to-run and day-to-day precisions for the corrected peak areas were calculated as 1.65 and 3.90 respectively. The applicability of the method has been demonstrated by analyzing acrylamide in the samples of potato chips and French fries. The method is simple, rapid, inexpensive, and widely applicable for the determination of acrylamide in food samples.

## Phycicochemical Features of Lanthanide-Alkali Metal Systems

**M. Gaune-Escard<sup>a</sup>, L. Rycerz<sup>b</sup>, E. Ingier-Stocka<sup>b</sup>, S. Gadzuric<sup>a,c</sup>**

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Lanthanide halide–alkali metal halide systems are very challenging from both a scientific and technological point of view.

When combined with alkali metal halides, lanthanide halides form different binary compounds in the solid state and complexes in liquids. Their existence and stability depend on the ionic radii of lanthanide, halide as well as alkali metal. Thus correlations were evidenced between thermodynamic and transport properties and ionic radii and structure both for pure lanthanide halides and their compounds with alkali metal halides. All these properties and their correlation are important also from a technological point of view.

Whatever the targeted technological application, basic knowledge is required for process development and optimization, in particular the thermodynamic and transport properties of lanthanide halides and their mixtures with alkali metal halides. However these data are scarce and not easily accessible in literature. As a consequence, intensive efforts are being made at an international level both on research and development aspects and also on data bank development.

# Unusual Phase Transitions in Complex Networks

**Michael Hinczewski**

*Feza Gursev Institute*

Recent years have seen a surge of interest in complex networks, which can describe systems as diverse as traffic on the world-wide web, metabolic interactions in cells, and the spread of epidemics among populations. From a statistical physics perspective, these networks provide an intriguing avenue for tackling one of the long-standing questions in the field: how the collective behavior of interacting objects is influenced by the topology of those interactions. In this talk, I will show how renormalization-group techniques can yield exact solutions for the Ising model---the canonical example of cooperative behavior---on a family of complex networks. Even for such a simple system the network structure leads to a variety of unusual thermodynamic behaviors: algebraic order, Berezinskii-Kosterlitz-Thouless phase transitions, and Griffiths singularities.

# Variable Morphologies of Styrene-co-perfluoroalkylethylacrylate Co- oligomers in Different Concentrations of THF

**Gökhan Kaçar, Alimet Sema Özen, Canan Atılğan**

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Block copolymers are known as self-organizing synthetic materials. In our study, Dissipative Particle Dynamics (DPD) simulation method is applied to styrene-co-perfluoroalkylethylacrylate (PFA) copolymer in tetrahydrofuran (THF) solvent system. These fluorocarbon oligomer systems form different micellar or lamellar morphologies in various concentrations. Dynamics of water on these surfaces consisting of the above morphologies is significantly important issue to study. To study these dynamics, different morphologies from DPD are obtained. System to be initially investigated has a PFA concentration of 5 % in copolymer and beads are aligned as A10B1D7 where A is styrene monomer, B is  $H_2C=(CH)-(C=O)-O-(CH_2)_2$  and D is  $CF_2-(CF_2)_5-CF_3$  parts of PFA monomer. Spherical micellar structure is obtained with 10 % styrene-co-PFA in THF solvent and cylindrical micellar structure is obtained with 80 % styrene-co-PFA in the same environment.

# **Bir-Boyutlu Schrödinger Denkleminin Geniş Bir Çözümler Kümesi**

**Bekir Karaoğlu**

*Haliç Üniversitesi, Fen-Edebiyat Fakültesi Uygulamalı Matematik Bölümü*

The number of potentials for which the Schrödinger equation could be solved analytically is limited. Or, the class of wavefunctions that satisfy the given boundary conditions can be extended infinitely, owing to a property of the Schrödinger equation. In this work, we explain the technique of increasing the number of analytical solutions and give sample solutions.

# Ground State Energy and Wigner Crystallization in Two-Dimensional Boson System

**A. I. Mese<sup>a</sup>, P. Capuzzi<sup>b</sup>, Z. Akdeniz<sup>c</sup>, S. E. Okan<sup>d</sup>, M. P. Tosi<sup>e</sup>**

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We study a rubidium gas of few atoms trapped by a harmonic potential, interacting via a logarithmic potential which is proper for two dimensional systems within the variational approximation. The ground state energy and density profile are calculated. The system is transformed into a fermion-like state from Bose-Einstein condensate if the strength of their interatomic repulsive interaction is increased. The Wigner molecule is established for  $N=2,3,6$  particles. Our results are in good agreement with the available via a coulombic potential.

# Structure and Stability of Molecular Clusters in Pentafluoride Compounds and Polymerization in Their Vapor Phase

**Z. Cicek Önem<sup>a</sup>, Z. Akdeniz<sup>a,b</sup> and M. P. Tosi<sup>b</sup>**

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<sup>b</sup> *Classe di Scienze, Scuola Normale Superiore, I-56126 Pisa, Italy*

Pentafluoride compounds such as NbF<sub>5</sub> and TaF<sub>5</sub> have been reported in the literature to admit various states of polymerization coexisting with monomers in their vapor phase, in relative concentrations that vary with temperature and pressure.

In this work we examine by means of an interionic force-field model the microscopic structure and the stability of a variety of isolated small clusters that may exist in the vapor phase of these compounds. The model, that was established by two of us [1] in a study of Al trichloride and alkali chloroaluminates, emulates the formation of chemical bonds by means of halogen polarizabilities accounting both for dipole induction by electric fields and for short-range overlap deformability of outer electron shells.

Our results are consistent with the findings of Boghosian et al. [2], indicating coexistence of monomers and dimers in vapors of these compounds, and broadly indicate that a variety of states of polymeric aggregation are allowed on static-energy grounds in these vapors.

[1] Z. Akdeniz and M. P. Tosi, *Z. Naturforsch.* 54a, 180 (1999).

[2] S. Boghosian, E. A. Pavlatou, and G. Papatheodorou, *Vibr. Spectr.* 37, 133 (2005).

# **Structure of Trivalent-Metal Halides Melts from Simulations based on Intramolecular Force Laws**

**Romina Ruberto**

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Diffraction studies of the liquid structure of **AlCl<sub>3</sub>**, **AlBr<sub>3</sub>**, **GaBr<sub>3</sub>** and **GaI<sub>3</sub>** close to their respective freezing points have revealed fourfold coordination of the trivalent metal ions, consistent with dimeric  $M_2X_6$  molecules being the dominant species.

We carry out classical molecular-dynamics simulations to examine how a polarizable-ion force law, determined on isolated molecular monomers and dimers in the gaseous phase of these compounds, accounts for the experimental data at a good quantitative level.

# Static Structure Factor of Glasses and Jammed Materials at Low Temperatures

Moises Silbert

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Recent Molecular Dynamics simulations of amorphous, or glassy, hard and soft spheres in the limit of very low temperatures has revealed that the asymptotic behaviour of the static structure factor,  $S(k)$ , in the long wavelength limit, is linear. It is important to note here that this limit, in the glassy phase at very low temperatures, is mainly dictated by the dynamics and not by thermal fluctuations.

After an introduction on glasses, granular materials, and the glass transition, as well as the Bose peak, the possible relationship between the small  $k$ -behaviour of  $S(k)$  and the Bose peak will be discussed.

# **Bhatia-Thornton Formalism for Multicomponent Mixtures**

**Moises Silbert**

*IFRN, Norwich Research Park, Colney Lane, Norwich, UK*

The extension of the Bhatia-Thornton formalism beyond fluid binary mixtures is not trivial. Here the extension to a three-component fluid mixture is presented, and then the three component ionic case is discussed. It is of interest to note that, in the latter, both charge and concentration fluctuations are present.

The specific case of a binary mixture of molten salts is illustrated for the liquid mixture  $(\text{AgI})_{0.3}(\text{AgBr})_{0.7}$ .

# **The Role of Confinement and Shape on the Binding Energy of an Electron in a Quantum Dot**

**S. Sucu<sup>a</sup>, A. İ. Meşe<sup>a</sup>, S. E. Okan<sup>b</sup>**

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The effect of both electric field and volume of structure on the impurity ground state binding energy in cubic and cylindrical GaAs/AlAs quantum dots is investigated using a variational procedure within the effective mass approximation. It is shown that the impurity ground state energy strongly depends on whether the confinement is along the electric field direction or perpendicular to it more than the shape of the dot.

# Temperature Dependence of the Tensile Properties of Carbon Nanotubes

Gülay Dereli, Banu Süngü

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Carbon nanotubes have the highest tensile strength of any material yet measured with labs producing them at a tensile strength of 63 Gpa that is still well below their theoretical limit of 300 Gpa. We report here on our recent investigations [1,2] on thermal characteristics of (10,10) Single-Walled Carbon Nanotubes (SWCNTs) using an O(N) TBMD simulation method that we previously developed [3,4,5].

We showed that SWCNTs keep their tensile strength in extension until very high temperatures up to 1800 K. They are not as strong in compression. We determined the high temperature positive/negative bond breaking strain values and stress-strain curves. We also focused on the effects of temperature increase on structural stability and the energetics of the tube. Through stress-strain curves, we obtained the Young's modulus and Poisson ratio values of (10,10) SWCNTs at elevated temperatures.

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[http://www.yildiz.edu.tr/~gdereli/lab\\_homepage/index.html](http://www.yildiz.edu.tr/~gdereli/lab_homepage/index.html)

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# Alternative Proton Conducting Membranes for High Temperature Fuel Cells

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Proton conducting membrane is a crucial part of Polymer Electrolyte Membrane Fuel Cells (PEMFC) and electrochromic devices. Standard membranes for PEM fuel cells are based on perfluorinated sulfonic acid copolymers (i.e., Nafion®). These membranes are unstable at higher temperatures and their proton conductivity sharply decreases near dew point of water. Considering also the relatively high cost, alternative membranes are the popular field of fuel cell research. In this study, recent advances on the anhydrous proton conducting blends based on basic or inert polymer/strong acid (i.e., phosphoric acid, sulfuric acid) and acidic polymer/heterocycle (i.e., imidazole, benzimidazole and pyrazole) are summarized.

Alternative anhydrous nafion blend membranes were synthesized doping triazole based heterocycle reagents. Methanol permeability measurements are performed with our homemade simple test cell. Anhydrous blend membranes showed lower methanol permeability compared to Nafion112. Proton conductivities were measured up to 180 °C under dry conditions. The results show that thermally stable, proton conducting membranes made by immobilizing triazole based reagents could be used in high temperature polymer electrolyte and direct methanol fuel cell systems.

**Keywords:** anhydrous proton conducting membrane, polymer electrolyte membrane, methanol permeability, proton conductivity, triazole

# Alginate-Polietilenimin-Kil Nanokompozitlerinin Eldesi ve Fiziksel Özelliklerinin İncelenmesi

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Son yıllarda killerin polimerler içinde nano boyutta dağılımının polimer yapısına çok belirgin fiziksel özellikler kazandırdığı bilinmekte ve farklı yapıda kil/polimer nanokompozitler üretilmektedir. Alginat; gluronik asit ile mannurik asitin bir kopolimeri olup, kahverengi deniz yosunundan izole edilerek saflaştırılan ve ticari olarak satılan bir polisakkarittir. Toksik özelliği olmayan, bioparçalanabilir, jel oluşturma özelliği olan ve suda çözünebilen bu polimerin gıda, ilaç ve biomedikal alanlarda(yara kapama, hepatokültür iskeleti oluşturma ve cerrahi müdahale gibi) çok geniş kullanım alanları mevcuttur. Polietilenimin ise su temizlenmesinden vücuda gen transferine kadar çeşitli biyolojik amaçlarla kullanılan; yine suda çözünen ve toksik olmayan bir polielektrolittir. Bu çalışmada çevre dostu üç komponentin alginat, polietilenimin (PEI) ve kilin nano boyutlarda birbirleri ile etkileşmesi sonucu oluşan kompozit ve film malzemeleri üretilmiş, malzemelerin optik ve termal özellikleri incelenmiştir.

# Temperature Dependence of the Energy Band Gaps of Carbon Nanotubes

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Tight-Binding Molecular Dynamics is successful in studying the structural, dynamical, and electronic properties of Single-Wall Carbon Nanotubes. In this study, order N parallel tight-binding molecular dynamics algorithms of (G. Dereli, C. Özdoğan, Phys. Rev. B. 67, 035415, 2003; G. Dereli, C. Özdoğan, Phys. Rev. B. 67, 035416, 2003; C. Özdoğan, G. Dereli, T. Çağın, Comput. Phys. Comm. 148, 2002) are used to study the band gaps of (10,0) SWCNT. This study is performed in Yıldız Technical University Carbon Nanotube Simulation Laboratory ([http://www.yildiz.edu.tr/~gdereli/lab\\_homepage/index.htm](http://www.yildiz.edu.tr/~gdereli/lab_homepage/index.htm)). We calculated the electronic density of states (eDOS), fermi energy level and band structure energy of (10,0) CNT as a function of temperature. We present the energy band gap variation of (10,0) semiconducting SWCNT with temperature. Using eDOS graphs we defined the band gap energies of (10,0) SWCNT. Our  $E_g(T) - E_g(0.1)$  values become more negative for larger T. We addressed the thermal expansion effects in the band gap in terms of the changes in the internal coordinates.