Prof. ZEKİ BÜYÜKMUMCU

Personal Information

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Education Information

Doctorate, Middle East Technical University, Graduate School Of Natural And Applied Sciences, Kimya, Turkey 1993 - 1998
Undergraduate, Middle East Technical University, Faculty Of Arts And Sciences, Kimya, Turkey 1985 - 1990

Research Areas

Basic Sciences, Chemistry, Physical Chemistry, Computational Chemistry, Conductive Polymers, Quantum Mechanics

Academic Titles / Tasks

Professor, Erciyes University, Fen Fakültesi, Kimya Bölümü, 2008 - Continues
Associate Professor, Erciyes University, Fen-Edebiyat Fakültesi, Kimya, 2002 - 2008
Assistant Professor, Erciyes University, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2001 - 2002
Research Assistant, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Chemistry, 1990 - 1999

Academic and Administrative Experience

2010 - Continues

Courses

Mesleki İngilizce II, Undergraduate, 2021 - 2022
General Chemistry I, Undergraduate, 2021 - 2022
Mesleki İngilizce I, Undergraduate, 2021 - 2022
Reaksiyon Kinetiği, Undergraduate, 2021 - 2022
Applied Mathematics for Physical Chemistry, Postgraduate, 2019 - 2020
Matematik, Undergraduate, 2016 - 2017
Malzeme Termodinamiği II, Undergraduate, 2016 - 2017
Matematik, Undergraduate, 2016 - 2017
Kimya I, Undergraduate, 2013 - 2014

Nükleer Kimya II, Undergraduate, 2013 - 2014
Elektrokimya, Undergraduate, 2013 - 2014
Fizikokimya Hesaplamaları, Postgraduate, 2013 - 2014
Physical Chemistry Calculations, Postgraduate, 2013 - 2014
Bitirme Tezi, Undergraduate, 2012 - 2013
Kuantum Kimyası, Undergraduate, 2012 - 2013
Fizikokimya II, Undergraduate, 2010 - 2011
Fizikokimya I, Undergraduate, 2010 - 2011
Kimyacılar için Bilgisayar Kullanımı, Undergraduate, 2010 - 2011
Genel Kimya Lab., Undergraduate, 2010 - 2011
Kinetik ve Kataliz, Undergraduate, 2009 - 2010
Kimyada Matematik Metotlar, Undergraduate, 2009 - 2010
Kimyasal Tepkime Dinamiği, Doctorate, 2008 - 2009
Radyokimya, Undergraduate, 2008 - 2009

Advising Theses

Büyükmumcu Z., Theoretical analysis of small fullerenes, Postgraduate, N.TAGHLIB(Student), 2019
Büyükmumcu Z., Bazı gümüş n-heterohalkalı karben komplekslerinin teorik analizi, Postgraduate, M.KALKAT(Student), 2018
BÜYÜKMUMCU Z., İLETKEN POLİMERLERDE HETEROATOM VE SUBSTİTUENT ETKİSİNİN TEORİK ANALİZİ, Postgraduate, İ.KOCATÜRK(Student), 2014
BÜYÜKMUMCU Z., SELENOLO [3,4B]SELENOFENİN ELEKTROKİMYASAL OLARAK OLİGOMERLEŞMESİNİN VE POLİSELENOLO [3,4B] SELENOFENİN BANT YAPISININ YOĞUNLUK FONKSİYONEL TEORİ İLE İNCELENMESİ, Postgraduate, D.DİLBAZ(Student), 2011
BÜYÜKMUMCU Z., Aseton–n-pentan Azeotropunun Farklı Kuramsal Metotlarla İncelenmesi, Postgraduate, İ.AYDIN(Student), 2008
BÜYÜKMUMCU Z., Aseton–n-hekzan Azeotropunun Farklı Kuramsal Metotlarla İncelenmesi, Postgraduate, S.KOLAY(Student), 2008
BÜYÜKMUMCU Z., Bazı Polimerlerin İletkenlik ve Titreşim Spektroskopik Özelliklerinin Kuramsal incelenmesi, Postgraduate, H.DA(Student), 2006
BÜYÜKMUMCU Z., Bazı Polimer Bileşiklerinin Titreşim Spektrumlarının Hesaplanması Amacıyla Kullanılan Hesaplama Yöntemlerinin Karşılaştırmalı İncelenmesi, Postgraduate, F.KÖSE(Student), 2005

Published journal articles indexed by SCI, SSCI, and AHCI

I. **Synthesis, spectral and theoretical (DFT) investigations of 4,6-diphenyl-6-hydroxy-1-{[(1Z)-1-phenyl ethylidene] amino}tetrahydropyrimidine-2(1H)-one**
ARI H., Ozpozan T., BÜYÜKMUMCU Z., Akin N., İLHAN İ. Ö.
JOURNAL OF MOLECULAR STRUCTURE, vol.1250, 2022 (SCI-Expanded)

II. **Revisiting UF6, NpF6 and PuF6 for bonding and molecular surface analysis within density functional theory: Comparative study at the different theory levels with the same basis set**
Buyukmumcu Z., Selampinar F.
POLYHEDRON, vol.209, 2021 (SCI-Expanded)

III. **Synthesis and thermal properties of magnetite nano structures and DFT analysis of Fe3O4 cluster as its smallest representative unit***
Pekdur Ö. S., Yıdırım S., BÜYÜKMUMCU Z.
Journal of Molecular Structure, vol.1222, 2020 (SCI-Expanded)

IV. **Synthesis and spectroscopic characterization and DFT study of benzyl 4-([1,1 '-biphenyl]-4-yl)-**

2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate
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JOURNAL OF MOLECULAR STRUCTURE, vol.1200, 2020 (SCI-Expanded)

V. **Redetermination and Density Functional Studies of N,N-(Disulfanediyldibenzene-2,1-Diyl) Dipyridine-2-Carboxamide**
YILDIRIM S., BÜYÜKMUMCU Z., Dogan S. D., Butcher R. J.
JOURNAL OF STRUCTURAL CHEMISTRY, vol.59, no.8, pp.1797-1803, 2018 (SCI-Expanded)

VI. **Redetermination and density functional studies of N,N'xx-(disulfanediyldibenzene-2,1-diyl)dipyridine-2-carboxamide**
Yıldırım S., Büyükmumcu Z., Doğan Ş. D., Butcher R. J.
Journal Of Structural Chemistry, vol.59, no.8, pp.1861-1867, 2018 (SCI-Expanded)

VII. **Electrochemical oligomerization of selenophene and band structure of polyselenophene: A density functional theory study**
Ari H., Mıhçıokur O., BÜYÜKMUMCU Z., MIHÇIOKUR H., ÖZPOZAN T.
COMPUTATIONAL MATERIALS SCIENCE, vol.154, pp.65-74, 2018 (SCI-Expanded)

VIII. **Vibrational spectroscopic study of isotopic effect on TcX3+ and TcX3OH (X: O, S and Se) by DFT**
Ari H., BÜYÜKMUMCU Z., ÖZPOZAN T.
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IX. **Synthesis, structural characterization and density functional studies of ethyl 4- (biphenyl-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate A nonmerohedral twinnedstructure**
YILDIRIM S., BÜYÜKMUMCU Z., Butcher R. J., Çetin G., Şİmşek R., Şafak C.
Journal Of Molecular Structure, vol.1163, no.7, pp.161-166, 2018 (SCI-Expanded)

X. **Comparison of DFT functionals for prediction of band gap of conjugated polymers and effect of HF exchange term percentage and basis set on the performance**
Ari H., BÜYÜKMUMCU Z.
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XI. **Theoretical analysis of TcO3(OH), TcS3(OH) and TcSe3(OH)**
BÜYÜKMUMCU Z.
JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY, vol.310, no.3, pp.1223-1231, 2016 (SCI-Expanded)

XII. **Theoretical and vibrational spectroscopic approach to keto-enol tautomerism in methy1-2-(4-methoxybenzoyl)-3-(4-methoxyphenyl)-3-oxopropanoylcarbamate**
Ari H., ÖZPOZAN T., BÜYÜKMUMCU Z., Kabacalı Y., Sacmaci M.
JOURNAL OF MOLECULAR STRUCTURE, vol.1122, pp.48-61, 2016 (SCI-Expanded)

XIII. **Vibrational and theoretical analysis of pentyl-4-benzoyl-1[2,4-dinitrophenyl]-5phenyl-1H-pyrazole-3-carboxylate**
Ari H., BÜYÜKMUMCU Z., ÖZPOZAN T., İLHAN I. Ö., BAHADIR O.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.110, pp.193-204, 2013 (SCI-Expanded)

XIV. **Poly(3,4-propylenedioxythiophene)s as a Single Platform for Full Color Realization**
Dey T., Invernale M. A., Ding Y., BÜYÜKMUMCU Z., Sotzing G. A.
MACROMOLECULES, vol.44, no.8, pp.2415-2417, 2011 (SCI-Expanded)

XV. **Poly(thieno[3,4-b]furan), a New Low Band Gap Polymer: Experiment and Theory**
Kumar A., Bokria J. G., BÜYÜKMUMCU Z., Dey T., Sotzing G. A.
MACROMOLECULES, vol.41, no.19, pp.7098-7108, 2008 (SCI-Expanded)

XVI. **Monte Carlo calculation of the de-excitation of fission fragments of Cf-252(sf) within multimodal random neck rupture model**
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KUMAR A., Buyukmumcu Z., SOTZING G.

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XVIII. **Vibrational spectra, normal coordinate treatment and simulation of the vibrational spectra of piperazine glyoxime and its Co(III) complex**
Ozpozan T., KÜÇÜKUSTA D., BÜYÜKMUMCU Z.
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XIX. **Ternary particle yields in Cf-249(n(th),f)**
Tsekhanovich I., Buyukmumcu Z., Davi M., Denschlag H., Gonnenwein F., BOULYGA S.
PHYSICAL REVIEW C, vol.67, no.3, 2003 (SCI-Expanded)

XX. **Mass and charge distributions in the very asymmetric mass region of the neutron induced fission of Np-238**
Tsekhanovich I., Denschlag H., Davi M., BÜYÜKMUMCU Z., Gonnenwein F., Oberstedt S., Faust H.
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XXI. **Mass and charge distributions in the very asymmetric thermal neutron induced fission of the odd-Z nucleus Am-242m**
Tsekhanovich I., Denschlag H. O., Davi M., BÜYÜKMUMCU Z., Wostheinrich M., Gonnenwein F., Oberstedt S., Faust H.
NUCLEAR PHYSICS A, vol.658, no.3, pp.217-239, 1999 (SCI-Expanded)

XXII. **Possible exit channel effect on isomer yield ratios**
Kildir M., Mörel Z., Buyukmumcu Z., Erten H. N.
JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY, vol.221, pp.161-165, 1997 (SCI-Expanded)

XXIII. **The diminution of the neutron odd-even effect due to prompt neutron emission in low energy nuclear fission**
BÜYÜKMUMCU Z., Kildir M.
JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY, vol.220, no.1, pp.27-30, 1997 (SCI-Expanded)

XXIV. **Determination of pre-scission kinetic energy in low energy fission using Isotonic Charge Distribution Model**
BÜYÜKMUMCU Z., Kildir M., Aras N. K.
JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY-ARTICLES, vol.204, no.2, pp.275-284, 1996 (SCI-Expanded)

XXV. **INFLUENCE OF EVEN NUCLEON NUMBERS AND CLOSED SHELLS ON MASS AND CHARGE-DISTRIBUTION IN LOW-ENERGY FISSION**
BÜYÜKMUMCU Z., ERTEN H. N., ARAS N. K.
JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY-ARTICLES, vol.181, no.1, pp.175-188, 1994 (SCI-Expanded)

Articles Published in Other Journals

I. **DFT Studies, Synthesis, Biological Activity And Crystal Structure of Tert-Butyl 4-([1,1′-Biphenyl]-4-Yl)-2-Methyl-5- Oxo-1,4,5,6,7,8-Hexahydroquinoline-3-Carboxylate**
YILDIRIM S., BÜYÜKMUMCU Z., Çetin G., ŞİMŞEK R., ŞAFAK O. C., Butcher R. J.
International Journal of Emerging Technology andAdvanced Engineering, vol.9, no.5, pp.1-7, 2019 (Peer-Reviewed Journal)

Books & Book Chapters

I. **Çekirdek Kimyası**
Büyükmumcu Z.
in: Kimya-Cilt 2, Mehmet TÜFEKÇİ,Serdar KARABÖCEK,Selami KARSLIOĞLU,Ahmet DEMİRBAŞ, Editor, Nobel Akademik Yayıncılık, Ankara, pp.934-969, 2014

II. **Bazı Kimyasal Tepkime Çeşitleri**

Büyükmumcu Z.
in: Kimya-Cilt 1, Mehmet TÜFEKÇİ,Serdar KARABÖCEK,Selami KARSLIOĞLU,Ahmet DEMİRBAŞ, Editor, Nobel Akademik Yayıncılık, Ankara, pp.211-244, 2014

III. **Applied Mathematics for Physical Chemistry**
Büyükmumcu Z.
Nobel Yayın Dağıtım, Ankara, 2009

Refereed Congress / Symposium Publications in Proceedings

I. **SYNTHESIS, CHARACTERIZATION, CRYSTAL STRUCTURE AND DFT ANALYSIS OF BENZYL 4-[2-FLUORO-4- (TRIFLUOROMETHYL)PHENYL]-2,6,6-TRIMETHYL1,4,5,6,7,8-HEXAHYDROQUINOLINE-3-CARBOXYLATE**
Çetin G., ŞİMŞEK R., YILDIRIM S., BÜYÜKMUMCU Z., Butcher R. J.
3rd International Gazi Pharma Symposium Series |, Ankara, Turkey, 08 September 2021, pp.140-141

II. **Conformational and Vibrational Spectroscopic Analysis of Elafibranor by DFT**
ARI H., ÖZPOZAN T., BÜYÜKMUMCU Z.
The 2nd International Congress on Advances in Bioscience and Biotechnology (ICABB), Podgorica, Serbia And Montenegro, 26 - 30 June 2018

III. **DFT Study of the Molecular Structure and Vibrational Analysis of Acadesine**
ARI H., ÖZPOZAN T., BÜYÜKMUMCU Z.
The 2nd International Congress on Advances in Bioscience and Biotechnology (ICABB), Podgorica, Serbia And Montenegro, 26 - 30 June 2018

IV. **DFT STUDIES, SYNTHESIS, BIOLOGICAL ACTIVITY AND CRYSTAL STRUCTURE OF TERT-BUTYL 4-([1,1?-BIPHENYL]-4-YL)-2-METHYL-5-OXO-1,4,5,6,7,8-HEXAHYDROQUINOLINE-3- CARBOXYLATE**
YILDIRIM S., BÜYÜKMUMCU Z., Çetin G., Şimşek R., Şafak C., Butcher R. J.
The International Conference on Material Science and Technology in Cappadocia (IMSTEC 2018), Nevşehir, Turkey, 17 - 19 September 2018, pp.289-294

V. **DFT Calculations on Structural and Spectroscopic Properties of 1-(5-(4-methoxyphenyl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one**
BÜYÜKMUMCU Z., ARI H., ÖZPOZAN T., Özdemir F., İLHAN İ. Ö.
International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2018), Ankara, Turkey, 26 - 27 April 2018

VI. **Assessment of DFT Functionals for Calculating Vibrational Frequencies of L-Amino Acids**
ARI H., ÖZPOZAN T., BÜYÜKMUMCU Z.
International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2018), Ankara, Turkey, 26 - 27 April 2018

VII. **N,3,5-triphenyl-4,5-dihydro-1H-pyrazole-1-carbox amide: Vibrational Spectroscopic Investigation and Quantum Chemical Calculations**
ÖZPOZAN T., ARI H., BÜYÜKMUMCU Z., AKIN N., İLHAN İ. Ö.
International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2018), Ankara, Turkey, 26 - 27 April 2018

VIII. **Vibrational Spectroscopic Investigation and DFT Studies on 4,6-diphenyl-6-hydroxy-1-{[(1Z)-1-phenyl ethylidene] amino}tetrahydropyrimidin-2(1H)-one**
ARI H., ÖZPOZAN T., BÜYÜKMUMCU Z., AKIN N., İLHAN İ. Ö.
International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2018), Ankara, Turkey, 26 - 27 April 2018

IX. **Structural and Spectral Analyses of N,N '-(2,2 '-Dithiodi-o-Phenylene)Bis-(Furan-2-Carboxamide)**
Yildirim S., BÜYÜKMUMCU Z., PEKDUR O. S., Butcher R. J., DOĞAN Ş. D.
33rd International Physics Congress of the Turkish-Physical-Society (TPS), Bodrum, Turkey, 6 - 10 September 2017, vol.1935

X. **Experimental and Molecular Modeling Investigation of Isopropyl 4-(Biphenyl-4-Yl)-2,6,6-Trimethyl-5-Oxo-1,4,5,6,7,8-Hexahydroquinoline-3-Carboxylate**
Yildirim S., Cetin G., BÜYÜKMUMCU Z., ŞİMŞEK R., Safak C., Butcher R. J., PAKDUR O. S.
33rd International Physics Congress of the Turkish-Physical-Society (TPS), Bodrum, Turkey, 6 - 10 September 2017, vol.1935

XI. **Experimental and Molecular Modeling Inverstigation of Isopropyl 4-(Biphenyl-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate**
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Turkish Physical Society 33rd International Physics Congress, 6 - 10 September 2017

XII. **structural and spectral analyses of N,N'xx-(2,2'xx-Dithiodi-o-phenylene) bis(furan-2-carboxamide)**
YILDIRIM S., BÜYÜKMUMCU Z., pekdur ö. s., butcher r., DOĞAN Ş. D.
http://tfd33.turkfizikdernegi.org, Muğla, Turkey, 6 - 10 September 2017

XIII. **Heteroatom Effect on the Band Gap of Five Membered Fused Bicyclic Polymers**
ÖZPOZAN T., ARI H., BÜYÜKMUMCU Z.
III. International Turkish Congress on Molecular Spectroscopy (TURCMOS 2017), 26 - 29 August 2017

XIV. **Time Dependent DFT Study of UV-Visible Spectrum of Polyselenophene Molecular Segment as a H2O Sensor**
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III. International Turkish Congress on Molecular Spectroscopy (TURCMOS2017), 26 - 29 September 2017

XV. **Systematic Vibrational Study of Saturated Chain Alcohols by DFT**
ARI H., ÖZPOZAN T., BÜYÜKMUMCU Z.
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XVI. **Isotopic Effect on Vibrational Spectroscopic Studies of TcX3 and TcX3OH (X: O, S and Se): A DFT Study**
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Büyükmumcu Z., Arı H., Özpozan T.
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XVIII. **Time Dependent Density Functional Theory Analysis of Substituent Effect on Electronic Excitation Energies of Fused Bicyclic Dimers**
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Arı H., BÜYÜKMUMCU Z.
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XX. **Evolution of Vibrational Spectrum during Oligomerization of Pyrrolo 3 4b pyrrole A DFT Study**
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XXI. **235U(n,f)'de Bölünme Ürünlerinde Nötron Yayımının ve Tek-Çift Etkisinin Monte Carlo Metoduyla Hesaplanması**
BÜYÜKMUMCU Z., KILDIR M., Aras N. K.
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XXII. **DFT Study of Substituent Effect on The Band Structure of Bicyclic Conjugated Polymer**
BÜYÜKMUMCU Z., Kocatürk İ.
32nd European Congress on Molecular Spectroscopy (EUCMOS 2014), Düsseldorf, Germany, 24 - 29 August 2014, pp.283

XXIII. **Time-Dependent Density Functional Study on Variation of UV-Visible Spectrum of Poly(phospolo[3,4b]phosphole) as a Function of Substituent**
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XXIV. **Theoretical Analysis of Substituent Effect on UV-Visible Spectrum of Poly(pyrrolo[3,4b]pyrrole)**
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International Turkish Congress on Molecular Spectroscopy, İstanbul, Turkey, 15 - 20 September 2013, pp.78

XXV. **Conformer Analysis of 4-Methyl-N-[2-Oxo-4-(4-Methylphenyl)-5-(4-Methylbenzoyl)pyrimidine-1(2H)-yl]Benzamide**
Aydın L., Şahan E., Özpozan T., Büyükmumcu Z., Önal Z.
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XXVI. **Conformer Analysis of 4 Methyl N 2 oxo 4 4 methylphenyl 5 4 methylbenzoyl pyrimidin 1 2H yl benzamide**
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XXVII. **Density Functional Theory Analysis of Isopentyl-4- benzoyl-1-[2,4-dinitrophenyl]-5-phenyl-1H-pyrazole -3- carboxylate**
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XXX. **Optically Transparent Conducting Polymers from Fused Heterocycles**
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XXXI. **Bazı Polimerlerin Elektrokimyasal Polimerizasyonunun DFT ve PM3 İle Karşılaştırılmalı İncelenmesi**
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XXXII. **Density Functional Theory Study of Geometry and Band Structure of Some Conducting Polymers**
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XXXVII. **Düşük Enerjili Nükleer Fisyonda Bölünme Öncesi Kinetik Enerjinin Belirlenmesi**
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VII. Ulusal Nükleer Bilimler ve Teknoloji Kongresi, İstanbul, Turkey, 3 - 06 September 1996

XXXVIII. **Düşük Enerjili Nükleer Fisyonda Çift-Tek Etkisi**
BÜYÜKMUMCU Z., ERTEN H. N., ARAS N. K.
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Congress and Symposium Activities

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