

## Prof. Dr. ŞAKİR ERKOÇ

### Kişisel Bilgiler

E-posta: erkoc@metu.edu.tr

Web: <https://avesis.metu.edu.tr/erkoc>

### Yönetilen Tezler

- ERKOÇ Ş., Investigation of InP and SiGe nanomaterials via molecular dynamics simulations, Doktora, N.NAYİR(Öğrenci), 2018
- ERKOÇ Ş., Investigation of structural and electronic properties of ZnCdTe ternary alloy nanostructures, Doktora, M.KURBAN(Öğrenci), 2016
- ERKOÇ Ş., Structural Properties of ZnO Binary Alloy Nanosystems: Molecular-Dynamics Simulations, Doktora, M.EMİN(Öğrenci), 2015
- SEZGİ N. A., ERKOÇ Ş., Investigation of structural properties of boron carbide nanosystems under mechanical and thermal effects: Molecular dynamics simulations, Doktora, Y.ŞİMŞEK(Öğrenci), 2014
- Yazıcıoğlu Y., Erkoç Ş., Investigation of structural properties of metal nanorods: Molecular dynamics simulations, Yüksek Lisans, H.YAĞLI(Öğrenci), 2014
- ERKOÇ Ş., Çeşitli nanoyapıların yapısal, elektronik ve manyetik özellikleri : molekül dinamiği benzetimleri ve yoğunluk fonksiyoneli kuramı hesapları, Doktora, A.Sholejh(Öğrenci), 2014
- ERKOÇ Ş., Structural,electronic and magnetic properties of various nanosystems: Molecular dynamics simulations and density functional theory calculations, Doktora, S.ALAEI(Öğrenci), 2014
- ERKOÇ Ş., SMMCON (m + n - 3) mikrotopaklarının yapısal, elektronik ve manyetik özellikleri : yoğunluk fonksiyoneli teorisi hesapları, Yüksek Lisans, N.KARA(Öğrenci), 2013
- ERKOÇ Ş., Structural, electronic, and magnetic properties of SmMCoN (M+N<3)microclusters: Density functional theory calculations, Yüksek Lisans, N.KARA(Öğrenci), 2013
- ERKOÇ Ş., Investigation of the structural properties of low dimensional nanostructures: Molecular dynamics simulations, Yüksek Lisans, B.ÖZDAMAR(Öğrenci), 2013
- AYDINOL M. K., ERKOÇ Ş., Investigation of the structural properties of silicene nanoribbons by molecular dynamics simulations, Yüksek Lisans, A.İNCE(Öğrenci), 2012
- ERKOÇ Ş., Acceleration of molecular dynamics simulation for TERSOFF2 potential through reconfigurable hardware, Yüksek Lisans, B.VARGÜN(Öğrenci), 2012
- GÜVENÇ YAZICIOĞLU A., ERKOÇ Ş., Structural properties of defected graphene nanoribbons under tension: Molecular-dynamics simulations, Yüksek Lisans, B.TÜZÜN(Öğrenci), 2012
- ERYILMAZ A., ERKOÇ Ş., Investigation of undergraduate students mental models about the quantization of physical observables, Doktora, D.NİLÜFER(Öğrenci), 2012
- ÖNAL I., ERKOÇ Ş., Quantum mechanical treatment of fullerene-based systems doped with various metal and non-metal elements as prospective spin-qubits, Yüksek Lisans, S.POLAD(Öğrenci), 2010
- ERKOÇ Ş., Biyolojik öneme sahip küçük moleküllerin kuantum kimyasal ve moleküler dinamik hesaplamalarla incelenmesi, Doktora, E.Deniz(Öğrenci), 2010
- ERKOÇ Ş., Quantum monte carlo methods for fermionic systems: Beyond the fixed-node approximation, Doktora, N.DUGAN(Öğrenci), 2010
- ERKOÇ Ş., Tailoring one dimensional novel nano structures for specific applications using tools of molecular modeling, Doktora, O.BARIŞ(Öğrenci), 2008
- ERKOÇ Ş., Nano sistemlerin hidrojen depolama kapasitesi: molecular-dinamik simülasyonları, Yüksek Lisans, A.Koyuncular(Öğrenci), 2008

ERKOÇ Ş., Interactions of lithium-carbon nanosystems: Molecular dynamics simulations and density functional theory calculations, Doktora, R.PEKÖZ(Öğrenci), 2008

ERKOÇ Ş., Hydrogen storage capacity of nanosystems: Molecular -dynamics simulations, Yüksek Lisans, A.KOYUNCULAR(Öğrenci), 2008

ERKOÇ Ş., Generation and simulations of nanostructures of cage structures, Doktora, E.TAŞCI(Öğrenci), 2007

ERKOÇ Ş., Structural properties of homonuclear and heteronuclear atomic clusters: Monte Carlo simulation study, Yüksek Lisans, N.DUGAN(Öğrenci), 2006

ERKOÇ Ş., Theoretical investigation of altini ternary clusters: Density functional theory calculations and molecular dynamics simulations, Doktora, H.OYMAK(Öğrenci), 2004

ERKOÇ Ş., AlTiNi üçlü topakların kuramsal olarak incelenmesi : yoğunluk fonksiyoneli kuramı hesapları ve moleküler dinamik simülasyonları, Doktora, H.Oymak(Öğrenci), 2004

ERKOÇ Ş., Stability of carbon nanotubes and nanorods under heat treatment: Molecular dynamics simulations, Yüksek Lisans, O.BARIŞ(Öğrenci), 2003

ERKOÇ Ş., Karbon nanotüp ve karbon nanoçubuk yapılarının sıcaklığa karşı dayanıklılığı : Moleküler- dinamik simülasyon metodu, Yüksek Lisans, O.Barış(Öğrenci), 2003

ERKOÇ Ş., Simulation of the casimir effect for various geometries, Yüksek Lisans, E.TAŞCI(Öğrenci), 2002

ERKOÇ Ş., Determination of minimum energy configuration of N equal point charges placed on an infinitely thin, conducting disk, Yüksek Lisans, H.OYMAK(Öğrenci), 2000

ERKOÇ Ş., Simulation of condenser microphone behavior, Yüksek Lisans, C.KIRBAŞ(Öğrenci), 1999

ERKOÇ Ş., Molecular dynamics simulation of water clusters, Yüksek Lisans, E.GÜNEYLER(Öğrenci), 1999

ERKOÇ Ş., Geometry optimization of small copper clusters: Monte Carlo simulation study, Yüksek Lisans, R.MOHAMMAD(Öğrenci), 1998

ERKOÇ Ş., Geometry optimization of small copper clusters: Monte Carlo simulations study., Yüksek Lisans, S.Rıad(Öğrenci), 1998

ERKOÇ Ş., Molecular-dynamics computer simulation of copper clusters:structural stability, energetics, and melting, Yüksek Lisans, C.Özdoğan(Öğrenci), 1996

ERKOÇ Ş., Molecular dynamics computer simulation f copper clusters: structural stability, energetics and melting, Yüksek Lisans, C.ÖZDOĞAN(Öğrenci), 1996

ERKOÇ Ş., Molecular-dynamics computer simulation of aluminium: Buik, surface and cluster properties, Doktora, Z.SUBHİ(Öğrenci), 1993

ERKOÇ Ş., Structural stability and energetics of carbon clusters:Tersoff empirical many-body potential energy function calculation, Yüksek Lisans, M.TÜRELİ(VİDAL)(Öğrenci), 1993

ERKOÇ Ş., Structural stability and energetics of carbon clusters:Tersoff emprirical many-body potential energy functon calculation, Yüksek Lisans, M.Türelİ(Vidal)(Öğrenci), 1993

ERKOÇ Ş., Molecular-dynamics computer simulation of aluminum: bulk, surface,and cluster properties, Doktora, Z.Subhi(Öğrenci), 1993

ERKOÇ Ş., Structural stability and energetics of P, S, and C microclusters, Yüksek Lisans, Y.TAHTAMONİ(Öğrenci), 1990

ERKOÇ Ş., Structural stability and energetics of selenium and tellurium microclusters:empirical many-body potential energy function calculation, Yüksek Lisans, A.ÜN LÜ(Öğrenci), 1990

ERKOÇ Ş., Self-consistent field calculations for the electronic properties of semiconductor superlattices, Yüksek Lisans, B.USLU(Öğrenci), 1988

ERKOÇ Ş., Development of a semi-empirical potential energy function: Applications to microclusters, Yüksek Lisans, Z.EL(Öğrenci), 1987

## SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- I. **Development of the ReaxFF Reactive Force Field for Inherent Point Defects in the Si/Silica System**  
Nayir N., van Duin A. C. T., ERKOÇ Ş.  
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.123, sa.19, ss.4303-4313, 2019 (SCI-Expanded)
- II. **Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its**

### **Application to GeO<sub>2</sub>/Ge Interfaces**

Nayir N., van Duin A. C. T., ERKOÇ Ş.

JOURNAL OF PHYSICAL CHEMISTRY C, cilt.123, sa.2, ss.1208-1218, 2019 (SCI-Expanded)

- III. **A density functional theory study on the structural and electronic properties of Pb<sub>x</sub>Sb<sub>y</sub>Se<sub>z</sub> (x plus y plus z=2, 3) clusters**  
Pekoz R., ERKOÇ Ş.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, cilt.32, sa.3, 2018 (SCI-Expanded)
- IV. **Segregation formation, thermal and electronic properties of ternary cubic CdZnTe clusters: MD simulations and DFT calculations**  
KURBAN M., ERKOÇ Ş.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.88, ss.243-251, 2017 (SCI-Expanded)
- V. **Mechanical properties of CdZnTe nanowires under uniaxial stretching and compression: A molecular dynamics simulation study**  
Kurban M., ERKOÇ Ş.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.122, ss.295-300, 2016 (SCI-Expanded)
- VI. **Structural Properties of Pristine and Defected ZnO Nanosheets Under Biaxial Strain: Molecular Dynamics Simulations**  
Kilic M. E., ERKOÇ Ş.  
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, cilt.16, sa.2, ss.1506-1516, 2016 (SCI-Expanded)
- VII. **Structural and thermal properties of Cd-Zn-Te ternary nanoparticles: Molecular-dynamics simulations**  
Kurban M., Malcioglu O. B., ERKOÇ Ş.  
CHEMICAL PHYSICS, cilt.464, ss.40-45, 2016 (SCI-Expanded)
- VIII. **The influence of instructional interactions on students' mental models about the quantization of physical observables: a modern physics course case**  
Korhasan N. D., ERYILMAZ A., ERKOC Ş.  
EUROPEAN JOURNAL OF PHYSICS, cilt.37, sa.1, 2016 (SCI-Expanded)
- IX. **Structural properties of indium phosphide nanorods: molecular dynamics simulations**  
Nayir N., TAŞCI E., ERKOÇ Ş.  
INTERNATIONAL JOURNAL OF NANOTECHNOLOGY, cilt.13, ss.809-831, 2016 (SCI-Expanded)
- X. **Structural and Electronic Properties of Zn<sub>m</sub>Cd<sub>n</sub>Te<sub>k</sub> (m plus n plus k=2-4) Clusters: DFT Calculations**  
Kurban M., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.12, sa.9, ss.2605-2615, 2015 (SCI-Expanded)
- XI. **Structural Properties of Monolayer Boron Carbide Nanoribbons Under Strain: Molecular Dynamics Simulations**  
Simsek Y., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.12, sa.9, ss.2180-2188, 2015 (SCI-Expanded)
- XII. **Structural and Thermal Properties of Indium Phosphide Nanoparticles: Molecular Dynamics Simulations**  
Nayir N., Tasci E. S., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.12, sa.9, ss.2134-2139, 2015 (SCI-Expanded)
- XIII. **Carbon Nanobuggy is Ready for a Test Drive!**  
Tasci E. S., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.12, sa.6, ss.1083-1085, 2015 (SCI-Expanded)
- XIV. **X-Doped (X = C, N, F, P) ZnO Sheet: Density Functional Theory Calculations**  
KÖKTEN H., ERKOÇ Ş.

- JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.12, sa.3, ss.395-398, 2015 (SCI-Expanded)
- XV. **Study of the Influence of Transition Metal Atoms on Electronic and Magnetic Properties of Graphyne Nanotubes Using Density Functional Theory**  
Alaei S., Jalili S., ERKOÇ Ş.  
FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES, cilt.23, sa.6, ss.494-499, 2015 (SCI-Expanded)
- XVI. **Investigating students' mental models about the quantization of light, energy, and angular momentum**  
Didis N., ERYILMAZ A., ERKOC Ş.  
PHYSICAL REVIEW SPECIAL TOPICS-PHYSICS EDUCATION RESEARCH, cilt.10, sa.2, 2014 (SCI-Expanded)
- XVII. **Structural properties of defected ZnO nanoribbons under uniaxial strain: Molecular dynamics simulations**  
Kilic M. E., ERKOÇ Ş.  
CURRENT APPLIED PHYSICS, cilt.14, sa.1, ss.57-67, 2014 (SCI-Expanded)
- XVIII. **Structural Properties of beta-Fe<sub>2</sub>O<sub>3</sub> Nanorods Under Strain: Molecular Dynamics Simulations**  
Alaei S., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.11, sa.1, ss.242-248, 2014 (SCI-Expanded)
- XIX. **Evolution of the electronic structure and properties of charged titanium doped aluminum nanoclusters**  
ERDOĞDU Y., ERKOÇ Ş.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.79, ss.599-610, 2013 (SCI-Expanded)
- XX. **Structural Properties of ZnO Nanotubes Under Uniaxial Strain: Molecular Dynamics Simulations**  
Kilic M. E., ERKOÇ Ş.  
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, cilt.13, sa.10, ss.6597-6610, 2013 (SCI-Expanded)
- XXI. **Structural Properties of ZnO Nanoparticles and Nanorings: Molecular Dynamics Simulations**  
Kilic M. E., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.10, sa.6, ss.1490-1496, 2013 (SCI-Expanded)
- XXII. **Molecular Dynamic Simulations of Pristine and Defective Graphene Nanoribbons Under Strain**  
Tuzun B., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.10, sa.2, ss.470-480, 2013 (SCI-Expanded)
- XXIII. **Structural Properties of Silicon Nanorods Under Strain: Molecular Dynamics Simulations**  
Ozdamar B., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.10, sa.1, ss.1-9, 2013 (SCI-Expanded)
- XXIV. **Molecular Dynamics Simulations of Zinc Oxide Nanostructures Under Strain: I-Nanoribbons**  
Kilic M. E., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.10, sa.1, ss.104-111, 2013 (SCI-Expanded)
- XXV. **Molecular Dynamics Simulations of ZnO Nanostructures Under Strain: II-Nanorods**  
Kilic M. E., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.10, sa.1, ss.112-118, 2013 (SCI-Expanded)
- XXVI. **GROUP 12 ELEMENTS AND THEIR SMALL CLUSTERS: ELECTRIC DIPOLE POLARIZABILITY OF Zn, Cd AND H-g, Zn-2 DIMER AND HIGHER Zn-n MICROCLUSTERS AND NEUTRAL, CATIONIC AND ANIONIC ZINC OXIDE MOLECULES (ZnO, ZnO+ AND ZnO-)**  
Oymak H., ERKOÇ Ş.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, cilt.26, sa.8, 2012 (SCI-Expanded)
- XXVII. **Molecular-dynamics simulations of silicene nanoribbons under strain**  
Ince A., ERKOÇ Ş.  
PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS, cilt.249, sa.1, ss.74-81, 2012 (SCI-Expanded)
- XXVIII. **Energetics and structural properties of carbon and oxygen doped hexagonal boron nitride sheets**  
KÖKTEN H., ERKOÇ Ş.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.44, sa.1, ss.215-217, 2011 (SCI-Expanded)
- XXIX. **Structural properties of boron carbide nanoparticles: Application of a new set of Stillinger-Weber**

## parameters

Dugan N., ERKOÇ Ş.

COMPUTATIONAL MATERIALS SCIENCE, cilt.50, sa.10, ss.2950-2954, 2011 (SCI-Expanded)

- XXX. **Investigation of Metal and Non-Metal Doped Dimer and Trimer C-60 Fullerene Chains as Prospective Spin Cluster Qubits**  
Polad S., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.8, sa.4, ss.694-706, 2011 (SCI-Expanded)
- XXXI. **Silicene nanoribbons: Molecular-dynamics simulations**  
Ince A., ERKOÇ Ş.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.50, sa.3, ss.865-870, 2011 (SCI-Expanded)
- XXXII. **Effects of Water Related Defects on Pentacene and Picene Molecules**  
Pekoz R., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.7, sa.10, ss.1889-1893, 2010 (SCI-Expanded)
- XXXIII. **Quantum chemical treatment of beta-sitosterol molecule**  
Kurban S., ERKOÇ F., ERKOÇ Ş.  
PHARMACEUTICAL BIOLOGY, cilt.48, sa.6, ss.637-642, 2010 (SCI-Expanded)
- XXXIV. **Density Functional Theory Calculations on Polyacene Molecules**  
Pekoz R., ERKOÇ Ş.  
ADVANCED SCIENCE LETTERS, cilt.3, sa.1, ss.43-48, 2010 (SCI-Expanded)
- XXXV. **On the SmCo Dimer: A Detailed Density Functional Theory Analysis**  
Oymak H., ERKOÇ Ş.  
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.114, sa.4, ss.1897-1905, 2010 (SCI-Expanded)
- XXXVI. **Quantum chemical investigation of nitrotyrosine (3-nitro-L-tyrosine) and 8-nitroguanine**  
ERKOÇ Ş., ERKOÇ F., SEPİCİ DİNÇEL A.  
AMINO ACIDS, cilt.38, sa.1, ss.319-327, 2010 (SCI-Expanded)
- XXXVII. **Structural and electronic features of the ubiquinone and ubiquinol molecules: molecular dynamics and quantum chemical treatments**  
Tekin E. D., ERKOÇ Ş.  
MOLECULAR SIMULATION, cilt.36, sa.10, ss.763-771, 2010 (SCI-Expanded)
- XXXVIII. **Structural and electronic properties of carbon-doped c-BN(110) surface**  
KÖKTEN H., ERKOÇ Ş.  
PHYSICA B-CONDENSED MATTER, cilt.404, ss.4937-4938, 2009 (SCI-Expanded)
- XXXIX. **A theoretical study of chemical doping and width effect on zigzag graphene nanoribbons**  
Pekoz R., ERKOÇ Ş.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.42, sa.2, ss.110-115, 2009 (SCI-Expanded)
- XL. **Quantum-chemical treatment of the linoleic acid molecule and two of its conjugated isomers**  
Kurban S., ERKOÇ F., ERKOÇ Ş.  
EUROPEAN JOURNAL OF LIPID SCIENCE AND TECHNOLOGY, cilt.111, sa.10, ss.1035-1041, 2009 (SCI-Expanded)
- XLI. **Analyzing Fe-Zn system using molecular dynamics, evolutionary neural nets and multi-objective genetic algorithms**  
Bhattacharya B., Kumar G. R. D., Agarwal A., ERKOÇ Ş., Singh A., Chakraborti N.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.46, sa.4, ss.821-827, 2009 (SCI-Expanded)
- XLII. **Structural and thermochemical properties, and energetics of C-8(NO<sub>2</sub>)(8) and C-20(NO<sub>2</sub>)(4n) (n=0-4)**  
Pekoez R., ERKOÇ Ş.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.46, sa.4, ss.849-853, 2009 (SCI-Expanded)
- XLIII. **A density functional theory study on the structures and energetics of C<sub>m</sub>Ten clusters (m + n ≤ 6)**  
Pekoz R., ERKOÇ Ş.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.45, sa.4, ss.912-920, 2009 (SCI-Expanded)
- XLIV. **Molecular Mechanics and Molecular Dynamics Simulations of Carbon Based Nanogears**

- Tasci E., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.4, ss.921-925, 2009 (SCI-Expanded)
- XLV. **Structural and Electronic Properties of GamSen Microclusters: Density Functional Theory Calculations**  
Pekoz R., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.4, ss.908-920, 2009 (SCI-Expanded)
- XLVI. **Structural, Electronic and Magnetic Properties of BN Nanotubes Doped with Mn and Cr: Exploring the Potential for Device Technology**  
KÖKTEN H., Ustunel H., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.4, ss.926-932, 2009 (SCI-Expanded)
- XLVII. **On the Possibility of a Polymer-Like Nanorod Based on Columnar Stacked Single Benzenoid Carbon Rings**  
MALCIOĞLU O. B., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.4, ss.903-907, 2009 (SCI-Expanded)
- XLVIII. **Enhancement of H-2 Storage in Carbon Nanotubes via Doping with a Boron Nitride Ring**  
Onay A. K., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.4, ss.933-941, 2009 (SCI-Expanded)
- XLIX. **A Special Issue on Physics and Chemistry of Nanoparticles**  
Erkoc S.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.4, ss.805, 2009 (SCI-Expanded)
- L. **Genetic algorithm-Monte Carlo hybrid geometry optimization method for atomic clusters**  
Dugan N., ERKOÇ Ş.  
COMPUTATIONAL MATERIALS SCIENCE, cilt.45, sa.1, ss.127-132, 2009 (SCI-Expanded)
- LI. **Endohedral Li/Li+ Doped Stone-Wales Defected Carbon Nanocapsules**  
Pekoez R., ERKOÇ Ş.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.6, sa.1, ss.30-40, 2009 (SCI-Expanded)
- LII. **Genetic Algorithm Application to the Structural Properties of Si-Ge Mixed Clusters**  
Dugan N., ERKOÇ Ş.  
MATERIALS AND MANUFACTURING PROCESSES, cilt.24, sa.3, ss.250-254, 2009 (SCI-Expanded)
- LIII. **Density functional theory study on the structural properties and energetics of Zn(m)Te(n) microclusters**  
Pekoez R., ERKOÇ Ş.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.40, sa.9, ss.2921-2930, 2008 (SCI-Expanded)
- LIV. **Quantum chemical calculations of warfarin sodium, warfarin and its metabolites**  
Tekin E. D. Ç., ERKOÇ F., YILDIZ İ., ERKOÇ Ş.  
COMMUNICATIONS IN COMPUTATIONAL PHYSICS, cilt.4, sa.1, ss.161-176, 2008 (SCI-Expanded)
- LV. **Quantum chemical treatment of Li/Li+ doped defected carbon nanocapsules**  
Pekoez R., ERKOÇ Ş.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.40, sa.8, ss.2752-2760, 2008 (SCI-Expanded)
- LVI. **Stability analysis of graphene nanoribbons by molecular dynamics simulations**  
Dugan N., ERKOÇ Ş.  
PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS, cilt.245, sa.4, ss.695-700, 2008 (SCI-Expanded)
- LVII. **Functionality of C(4,4) carbon nanotube as molecular detector**  
MALCIOĞLU O. B., ERKOÇ Ş.  
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, cilt.8, sa.2, ss.469-478, 2008 (SCI-Expanded)
- LVIII. **Li+ and Li interactions with carbon nanocage structures**  
Pekoez R., ERKOÇ Ş.  
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, cilt.8, sa.2, ss.675-678, 2008 (SCI-Expanded)
- LIX. **Structural properties and stability of nanoclusters**  
Ustunel H., Erkoc S.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.4, sa.5, ss.928-956, 2007 (SCI-Expanded)

- LX. **Structural and electronic properties of defected carbon nanocapsules**  
 Pekoez R., Erkoc S.  
 JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, cilt.4, sa.4, ss.764-771, 2007 (SCI-Expanded)
- LXI. **An algorithm for constructing various kinds of nanojunctions using zig-zag and armchair nanotubes**  
 Tasci E., Erkoc S.  
 JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, cilt.7, ss.1653-1661, 2007 (SCI-Expanded)
- LXII. **Evolutionary and genetic algorithms applied to Li+-C system: Calculations using differential evolution and particle swarm algorithm**  
 Chakraborti N., Jayakanth R., Das S., Calisir E. A., Erkoc S.  
 JOURNAL OF PHASE EQUILIBRIA AND DIFFUSION, cilt.28, sa.2, ss.140-149, 2007 (SCI-Expanded)
- LXIII. **Structural and electronic properties of lithium endohedral doped carbon nanocapsules**  
 Pekoz R., Erkoc S.  
 PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.36, sa.2, ss.211-216, 2007 (SCI-Expanded)
- LXIV. **Thermal Stability of Carbon Nanosystems: Molecular-Dynamics Simulations**  
 Erkoc S., MALCIOĞLU O. B., TAŞCI E.  
 NANOMATERIALS: DESIGN AND SIMULATION, cilt.18, ss.201-226, 2007 (SCI-Expanded)
- LXV. **Genetic algorithms applied to Li+ ions contained in carbon nanotubes: An investigation using particle swarm optimization and differential evolution along with molecular dynamics**  
 Chakraborti N., Das S., Jayakanth R., Pekoz R., Erkoc S.  
 MATERIALS AND MANUFACTURING PROCESSES, cilt.22, ss.562-569, 2007 (SCI-Expanded)
- LXVI. **Structural, electronic and QSAR properties of the cyfluthrin molecule: A theoretical AM1 and PM3 treatment**  
 Calisir E. D., Erkoc S.  
 INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.17, sa.10, ss.1391-1402, 2006 (SCI-Expanded)
- LXVII. **Density functional theory calculations for [C<sub>2</sub>H<sub>4</sub>N<sub>2</sub>O<sub>6</sub>](n) (n=0,+1,-1)**  
 Turker L., Erkoc S.  
 JOURNAL OF HAZARDOUS MATERIALS, cilt.136, sa.2, ss.164-169, 2006 (SCI-Expanded)
- LXVIII. **Structural and electronic properties of dipropyl sulfide: A theoretical investigation**  
 Calisir E. D., Erkoc S.  
 INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.17, sa.8, ss.1179-1190, 2006 (SCI-Expanded)
- LXIX. **Structural properties of copper nanoparticles: Modified diffusion Monte Carlo simulations**  
 Dugan N., Erkoc S.  
 INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.17, sa.8, ss.1171-1177, 2006 (SCI-Expanded)
- LXX. **Comment on 'Modelling complexes of H-2 molecules in fullerenes' by H. Dodziuk [Chem. Phys. Lett. 410 (2005) 39]**  
 Turker L., Erkoc S.  
 CHEMICAL PHYSICS LETTERS, cilt.426, ss.222-223, 2006 (SCI-Expanded)
- LXXI. **Polarizabilities and second hyperpolarizabilities of ZnMcdn clusters**  
 Papadopoulos M. G., Reis H., Avramopoulos A., Erkoc S., Amirouche L.  
 MOLECULAR PHYSICS, cilt.104, ss.2027-2036, 2006 (SCI-Expanded)
- LXXII. **Structural and electronic properties of the DPPC molecule**  
 Erkoc S., Korkmaz F.  
 INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.17, sa.7, ss.967-974, 2006 (SCI-Expanded)
- LXXIII. **Structural and electronic properties of c-BN(110) surface and surface point defects**  
 Kokten H., Erkoc S.  
 INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.17, sa.6, ss.795-803, 2006 (SCI-Expanded)
- LXXIV. **Structural and electronic properties of bamboo-like carbon nanostructure**  
 Erkoc S.  
 PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.31, sa.1, ss.62-66, 2006 (SCI-Expanded)
- LXXV. **Metal atom endohedrally doped C-20 cage structure: (X@C-20; X = Ni, Fe, Co)**  
 Erkoc S.

- INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.16, sa.10, ss.1553-1560, 2005 (SCI-Expanded)
- LXXVI. **Structural and electronic properties of single-wall ZnO nanotubes**  
Erkoc S., Kokten H.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.28, sa.2, ss.162-170, 2005 (SCI-Expanded)
- LXXVII. **Quantum chemical investigation of thalidomide molecule**  
Erkoc S., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.719, ss.1-5, 2005 (SCI-Expanded)
- LXXVIII. **Correlations between the energetics of ZnCd nanoparticles and some of their corresponding bulk properties: molecular-dynamics simulations**  
Amirouche L., ERKOÇ Ş.  
JOURNAL OF CRYSTAL GROWTH, cilt.275, 2005 (SCI-Expanded)
- LXXIX. **Theoretical investigation of sulforaphane molecule**  
Erkoc S., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.714, ss.81-85, 2005 (SCI-Expanded)
- LXXX. **Theoretical investigations of the equol molecule: semi-empirical and density functional theory calculations**  
Erkoc F., Yilmazer M., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.713, ss.37-42, 2005 (SCI-Expanded)
- LXXXI. **Cluster, surface and bulk properties of ZnCd binary alloys: Molecular-dynamics simulations**  
Erkoc S.  
NEW FRONTIERS OF PROCESSING AND ENGINEERING IN ADVANCED MATERIALS, cilt.502, ss.51-56, 2005 (SCI-Expanded)
- LXXXII. **Density functional theory calculations for mercury fulminate**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.712, ss.139-142, 2004 (SCI-Expanded)
- LXXXIII. **Does tubular structure of carbon form only from graphine sheet?**  
Erkoc S.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.25, sa.1, ss.69-77, 2004 (SCI-Expanded)
- LXXXIV. **Structure and electronic properties of heterofullerene C30B15N15**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.684, ss.117-120, 2004 (SCI-Expanded)
- LXXXV. **Semi-empirical SCF-MO calculations for the structural and electronic properties of single-wall InP nanotubes**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.676, ss.109-113, 2004 (SCI-Expanded)
- LXXXVI. **A comparative study of empirical potential energy functions: Applications to silicon microclusters**  
Erkoc S., Takahashi K.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.15, sa.3, ss.403-408, 2004 (SCI-Expanded)
- LXXXVII. **Molecular-dynamics simulations of surface and bulk properties of Zn, Cd, and ZnCd systems**  
Amirouche L., Erkoc S.  
PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS, cilt.241, sa.2, ss.292-297, 2004 (SCI-Expanded)
- LXXXVIII. **A study of the Cu clusters using gray-coded genetic algorithms and differential evolution**  
Chakraborti N., Mishra P., Erkoc S.  
JOURNAL OF PHASE EQUILIBRIA AND DIFFUSION, cilt.25, sa.1, ss.16-21, 2004 (SCI-Expanded)
- LXXXIX. **Structural and energetic features of Al<sub>n</sub>Tin<sub>n</sub> (n=1-16) nanoparticles: molecular-dynamics simulations**  
Oymak H., Erkoc S.  
MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING, cilt.12, sa.1, ss.109-120, 2004 (SCI-Expanded)
- XC. **Ammonia deposition in fullerene: (NH<sub>3</sub>)(n) @C-60**  
Erkoc S., Turker L.



- JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.640, ss.57-61, 2003 (SCI-Expanded)
- XCI. **AlTiNi ternary alloy clusters: Molecular dynamics simulations and density functional theory calculations**  
Erkoc S., Oymak H.  
JOURNAL OF PHYSICAL CHEMISTRY B, cilt.107, sa.44, ss.12118-12125, 2003 (SCI-Expanded)
- XCII. **AM1 treatment of endohedrally hydrogen doped fullerene, nH(2)@C-60**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.638, ss.37-40, 2003 (SCI-Expanded)
- XCIII. **AMI treatment of substitutionally Al and P doped cyclacenes**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.637, ss.189-193, 2003 (SCI-Expanded)
- XCIV. **Structural features and energetics of Znn-mCdm (n=7,8) microclusters and Zn-50, Cd-50, and Zn25Cd25 nanoparticles: Molecular-dynamics simulations**  
Amirouche L., Erkoc S.  
PHYSICAL REVIEW A, cilt.68, sa.4, 2003 (SCI-Expanded)
- XCV. **AM1 treatment of substitutionally Al and P doped cyclacenes**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.636, ss.143-147, 2003 (SCI-Expanded)
- XCVI. **Structural and electronic properties of endofullerenes X@C-60**  
Erkoc S., Turker L.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.634, ss.195-199, 2003 (SCI-Expanded)
- XCVII. **Resveratrol and its analogues resveratrol-dihydroxyl isomers: semi-empirical SCF-MO calculations**  
Erkoc S., Keskin N., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.631, ss.67-73, 2003 (SCI-Expanded)
- XCVIII. **Structural and electronic properties of ajoene molecule**  
Erkoc S., Sumer S., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.631, ss.271-276, 2003 (SCI-Expanded)
- XCIX. **Theoretical investigation of hydroxytyrosol and its radicals**  
Erkoc F., Keskin N., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.625, ss.87-94, 2003 (SCI-Expanded)
- C. **Structural and electronic properties of magnesium diboride**  
Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.14, sa.4, ss.483-489, 2003 (SCI-Expanded)
- CI. **Structural and electronic properties of neodymium diiodide**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.623, ss.79-81, 2003 (SCI-Expanded)
- CII. **A theoretical study on certain iron-sulfur and iron-selenium clusters**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.623, ss.17-21, 2003 (SCI-Expanded)
- CIII. **Structural and electronic properties of ZnmCdn microclusters: density functional theory calculations**  
Erkoc S.  
CHEMICAL PHYSICS LETTERS, cilt.369, ss.605-609, 2003 (SCI-Expanded)
- CIV. **Application of genetic algorithms to geometry optimization of microclusters: A comparative study of empirical potential energy functions for silicon**  
Erkoc S., Leblebicioglu K., Halici U.  
MATERIALS AND MANUFACTURING PROCESSES, cilt.18, sa.3, ss.329-339, 2003 (SCI-Expanded)
- CV. **Structural and electronic properties of AlkTiINim microclusters: Density-functional-theory calculations**  
Oymak H., Erkoc S.  
PHYSICAL REVIEW A, cilt.66, sa.3, 2002 (SCI-Expanded)
- CVI. **Simulation of the Casimir-Polder effect for various geometries**

- Tasci E, Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.13, sa.7, ss.979-985, 2002 (SCI-Expanded)
- CVII. **Structural and electronic properties of guanine and guanosine**  
Erkoc F., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.589, ss.405-411, 2002 (SCI-Expanded)
- CVIII. **Gold deposition on GaAs(001) surfaces: Molecular-dynamics simulations**  
Erkoc S, Amirouche L, Rouaiguia L.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.13, sa.6, ss.759-769, 2002 (SCI-Expanded)
- CIX. **Decomposition of SiH<sub>4</sub> on the S-A type stepped Si(100) surface**  
Katircioglu S., Erkoc S.  
SURFACE REVIEW AND LETTERS, cilt.9, ss.1401-1407, 2002 (SCI-Expanded)
- CX. **Structural and electronic properties of porphyrin skeleton of chlorophyll**  
Erkoc S., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.579, ss.41-44, 2002 (SCI-Expanded)
- CXI. **Stability of carbon nanoion C-20@C-60@C-240: Molecular dynamics simulations**  
Erkoc S.  
NANO LETTERS, cilt.2, sa.3, ss.215-217, 2002 (SCI-Expanded)
- CXII. **Structural and electronic properties of rubreneperoxides**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.578, ss.99-101, 2002 (SCI-Expanded)
- CXIII. **Borazine embedded cyclacenes-MINDO3 treatment**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.578, ss.65-69, 2002 (SCI-Expanded)
- CXIV. **Electronic properties of open-ended single wall carbon nanotubes**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.577, ss.131-135, 2002 (SCI-Expanded)
- CXV. **Interaction of nitric oxide with elements**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.574, ss.127-132, 2001 (SCI-Expanded)
- CXVI. **Energetics and stability of discrete charge distribution on a conducting disk**  
Erkoc S., Oymak H.  
PHYSICS LETTERS A, cilt.290, ss.28-34, 2001 (SCI-Expanded)
- CXVII. **Structural and electronic properties of carbon nanoballs: C-20, C-60, and C-20@C-60**  
Erkoc S., Turker L.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.12, sa.9, ss.1391-1399, 2001 (SCI-Expanded)
- CXVIII. **Structural and electronic properties of PFOS and LiPFOS**  
Erkoc S., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.549, sa.3, ss.289-293, 2001 (SCI-Expanded)
- CXIX. **Structural and electronic properties of HEME and HEME-X; X = O-2, CO, NO**  
Erkoc S., Erkoc F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.546, ss.175-181, 2001 (SCI-Expanded)
- CXX. **Adsorption of water on single and double layer stepped Si(100) surfaces**  
Katircioglu S., Salman S., Erkoc S.  
SURFACE REVIEW AND LETTERS, cilt.8, ss.251-259, 2001 (SCI-Expanded)
- CXXI. **Optical transitions in parabolic GaAs/Ga<sub>1-x</sub>Al<sub>x</sub>As superlattices**  
Erkoc S., Kokten H.  
SURFACE REVIEW AND LETTERS, cilt.8, ss.321-325, 2001 (SCI-Expanded)
- CXXII. **Adsorption of hydrogen and oxygen on single and double layer stepped Si(100) surfaces**  
Salman S., Katircioglu S., Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, cilt.15, sa.16, ss.2261-2274, 2001 (SCI-Expanded)
- CXXIII. **Structural and electronic properties of single-wall BN nanotubes**

- Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.542, ss.89-93, 2001 (SCI-Expanded)
- CXXIV. **Structural and electronic properties of MTA**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.542, ss.95-99, 2001 (SCI-Expanded)
- CXXV. **Structural and electronic properties of InmSen microclusters: density functional theory calculations**  
Erkoc S, Katircioglu S., Yilmaz T.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.542, ss.101-105, 2001 (SCI-Expanded)
- CXXVI. **Molecular-dynamics simulations of carbon nanocage structures: Nanoballs and nanotoroids**  
Erkoc S., Vural D.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.12, sa.5, ss.685-690, 2001 (SCI-Expanded)
- CXXVII. **Structural and electronic properties of borazine cyclacenes**  
Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.540, ss.153-156, 2001 (SCI-Expanded)
- CXXVIII. **Structural and electronic properties of halogenated coronene**  
Erkoc S., Erkoc F., Turker L.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.538, ss.91-97, 2001 (SCI-Expanded)
- CXXIX. **Fragmentation of water clusters: Molecular-dynamics simulation study**  
Erkoc S., Kokten H., Guvenc Z.  
EUROPEAN PHYSICAL JOURNAL D, cilt.13, sa.3, ss.361-365, 2001 (SCI-Expanded)
- CXXX. **Electronic band structure of stepped Si(100) surfaces**  
Salman S., Katircioglu S., Erkoc S.  
SURFACE REVIEW AND LETTERS, cilt.8, ss.61-66, 2001 (SCI-Expanded)
- CXXXI. **Structural and electronic properties of bare and hydrogenated silicon clusters**  
Katircioglu S., Erkoc S.  
PHYSICA E, cilt.9, sa.2, ss.314-320, 2001 (SCI-Expanded)
- CXXXII. **Energetics and stability of discrete charge distribution on the surface of a sphere**  
Oymak H., Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.12, sa.2, ss.293-305, 2001 (SCI-Expanded)
- CXXXIII. **Structural and electronic properties of perchlorocoronene**  
Erkoc S., Erkoc F., Turker L.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.535, ss.159-164, 2001 (SCI-Expanded)
- CXXXIV. **Molecular-dynamics simulations of gold clusters**  
Bastug T., Hirata M., Varga S., Fricke B., Erkoc S., Mukoyama T.  
ADVANCES IN QUANTUM CHEMISTRY, VOL 37, cilt.37, ss.353-364, 2001 (SCI-Expanded)
- CXXXV. **Melting and fragmentation of nickel nanoparticles: Molecular-dynamics simulations**  
Gunes B., Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.8, ss.1567-1580, 2000 (SCI-Expanded)
- CXXXVI. **Borazine embedded cyclacenes - a theoretical study**  
Turker L., Erkoc S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.531, ss.401-405, 2000 (SCI-Expanded)
- CXXXVII. **Rules for the distribution of point charges on a conducting disk**  
Erkoc S., Oymak H.  
PHYSICAL REVIEW E, cilt.62, sa.3, 2000 (SCI-Expanded)
- CXXXVIII. **Energetics of arsenic terminated GaAs(001) surfaces**  
Erkoc S., Kokten H.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.6, ss.1225-1237, 2000 (SCI-Expanded)
- CXXXIX. **Zirconium microclusters: molecular-dynamics simulations and density functional calculations**  
Bastug T., Erkoc S., Hirata M., Tachimori S.  
PHYSICA E, cilt.8, sa.3, ss.223-229, 2000 (SCI-Expanded)
- CXL. **From carbon nanotubes to carbon nanorods**

- Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.6, ss.1247-1255, 2000 (SCI-Expanded)
- CXLI. **Stability of gold clusters: molecular-dynamics simulations**  
Erkoc S.  
PHYSICA E, cilt.8, sa.3, ss.210-218, 2000 (SCI-Expanded)
- CXLII. **General analytic density distribution function for atoms**  
Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.6, ss.1167-1177, 2000 (SCI-Expanded)
- CXLIII. **Molecular-dynamics simulation of stepped Si(100) surface**  
Katircioglu S., Salman S., Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.5, ss.999-1011, 2000 (SCI-Expanded)
- CXLIV. **Molecular-dynamics simulations of water clusters**  
Erkoc S., Guneyler E.  
PHYSICA E, cilt.8, sa.1, ss.40-49, 2000 (SCI-Expanded)
- CXLV. **Decomposition of C-60 molecules on Si(100)(2 x 1) surface**  
Erkoc S., Katircioglu S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.5, ss.1067-1076, 2000 (SCI-Expanded)
- CXLVI. **Molecular-dynamics simulations of nickel clusters**  
Erkoc S., Gunes B., Gunes P.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.5, ss.1013-1024, 2000 (SCI-Expanded)
- CXLVII. **Molecular-dynamics simulation of radiation damage on copper clusters**  
Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.5, ss.1025-1032, 2000 (SCI-Expanded)
- CXLVIII. **Energetics and stability of small SimCn clusters: AM1 and PM3 calculations**  
Erkoc S., Turker L.  
PHYSICA E, cilt.8, sa.1, ss.50-56, 2000 (SCI-Expanded)
- CXLIX. **Distribution of point charges on a thin conducting disk**  
Oymak H., Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.5, ss.891-900, 2000 (SCI-Expanded)
- CL. **A comparative study of empirical potential energy functions: Applications to clusters**  
Gunes P., Simsek S., Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.3, ss.451-467, 2000 (SCI-Expanded)
- CLI. **The effect of PBC on the simulation of nanotubes**  
Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.3, ss.547-551, 2000 (SCI-Expanded)
- CLII. **Structural and electronic properties of carbon nanotubes**  
Erkoc S.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, cilt.11, sa.1, ss.175-182, 2000 (SCI-Expanded)
- CLIII. **Energetics and structural stability of lanthanum microclusters**  
Erkoc S., Bastug T., Hirata M., Tachimori S.  
CHEMICAL PHYSICS LETTERS, cilt.314, ss.203-209, 1999 (SCI-Expanded)
- CLIV. **Monte Carlo computer simulation of copper clusters**  
Erkoc S., Shaltaf R.  
PHYSICAL REVIEW A, cilt.60, sa.4, ss.3053-3057, 1999 (SCI-Expanded)
- CLV. **Atomic and electronic properties of spherical silicon clusters**  
Erkoc S., Katircioglu S.  
PHYSICA E, cilt.4, sa.3, ss.185-191, 1999 (SCI-Expanded)
- CLVI. **Electronic structure of carbon nanotubes: AM1-RHF calculations**  
Erkoc S., Turker L.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, cilt.4, sa.3, ss.192-195, 1999 (SCI-Expanded)
- CLVII. **Application of density-functional theory to atomic resonances**

- Erkoc S., Jansen H.  
PHYSICAL REVIEW A, cilt.59, sa.3, ss.2490-2493, 1999 (SCI-Expanded)
- CLVIII. **Molecular-dynamics simulations of uranium microclusters**  
Erkoc S., Bastug T., Hirata M., Tachimori S.  
JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN, cilt.68, sa.2, ss.440-445, 1999 (SCI-Expanded)
- CLIX. **Energetics of carbon nanotubes**  
Erkoc S., Ozkaymak S.  
EUROPEAN PHYSICAL JOURNAL D, cilt.4, sa.3, ss.331-333, 1998 (SCI-Expanded)
- CLX. **Dependence of energy levels and optical transitions on layer thicknesses in InSe/GaSe superlattices**  
Erkoc S., Katircioglu S.  
JOURNAL OF CRYSTAL GROWTH, cilt.194, ss.331-335, 1998 (SCI-Expanded)
- CLXI. **Optical transitions in InSe/GaSe superlattices**  
Katircioglu S., Erkoc S., Allahverdi K.  
THIN SOLID FILMS, cilt.323, ss.194-198, 1998 (SCI-Expanded)
- CLXII. **An atomistic study on the stretching of nanowires**  
Mehrez H., Ciraci S., Fong C., Erkoc S.  
JOURNAL OF PHYSICS-CONDENSED MATTER, cilt.9, sa.49, ss.10843-10854, 1997 (SCI-Expanded)
- CLXIII. **Molecular-dynamics simulation of the structural stability, energetics, and melting of Cu-n(n=13-135) clusters**  
Ozdogan C., Erkoc S.  
ZEITSCHRIFT FUR PHYSIK D-ATOMS MOLECULES AND CLUSTERS, cilt.41, sa.3, ss.205-209, 1997 (SCI-Expanded)
- CLXIV. **Adsorption of H<sub>2</sub>O on double layer stepped Si(111) surface**  
Katircioglu S., Erkoc S.  
SURFACE SCIENCE, cilt.374, ss.208-214, 1997 (SCI-Expanded)
- CLXV. **Optical transitions in Si/Ge superlattices**  
Erkoc S., Katircioglu S.  
THIN SOLID FILMS, cilt.295, ss.206-209, 1997 (SCI-Expanded)
- CLXVI. **Investigation of HMO spectra of Huckel and Mobius type cyclacenes**  
Turker L., Erkoc S.  
TURKISH JOURNAL OF CHEMISTRY, cilt.21, sa.3, ss.167-172, 1997 (SCI-Expanded)
- CLXVII. **Empirical many-body potential energy functions used in computer simulations of condensed matter properties**  
Erkoc S.  
PHYSICS REPORTS-REVIEW SECTION OF PHYSICS LETTERS, cilt.278, sa.2, ss.80-105, 1997 (SCI-Expanded)
- CLXVIII. **Water adsorption on the stepped Si(110) surface**  
Katircioglu S., Erkoc S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.196, sa.1, ss.77-84, 1996 (SCI-Expanded)
- CLXIX. **AN EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION CONSTRUCTED FROM PAIR-INTERACTIONS**  
ERKOC S.  
ZEITSCHRIFT FUR PHYSIK D-ATOMS MOLECULES AND CLUSTERS, cilt.32, sa.3, ss.257-260, 1994 (SCI-Expanded)
- CLXX. **ELECTRONIC STATES OF INSE GASE SUPERLATTICE**  
ERKOC S., ALLAHVERDI K., IBRAHIM Z.  
SOLID STATE COMMUNICATIONS, cilt.90, sa.9, ss.553-556, 1994 (SCI-Expanded)
- CLXXI. **ADSORPTION SITES OF GE ADATOMS ON STEPPED SI(110) SURFACE**  
KATIRCIOGLU S., ERKOC S.  
SURFACE SCIENCE, cilt.311, sa.3, 1994 (SCI-Expanded)
- CLXXII. **DEPENDENCE OF RESONANCE STATES ON DOPING LEVEL AND DOPING DISTRIBUTION TYPE IN GAAS GA<sub>0.75</sub>AL<sub>0.25</sub>AS SUPERLATTICE**  
KATIRCIOGLU S., ERKOC S.  
SURFACE SCIENCE, cilt.311, 1994 (SCI-Expanded)

- CLXXIII. **BULK AND SURFACE-PROPERTIES OF ALUMINUM - A MOLECULAR-DYNAMICS SIMULATION**  
ELBAYYARI Z., ERKOC S.  
MATERIALS CHEMISTRY AND PHYSICS, cilt.37, sa.4, ss.382-388, 1994 (SCI-Expanded)
- CLXXIV. **EMPIRICAL TIGHT-BINDING TOTAL ELECTRONIC-ENERGY CALCULATION FOR  $\text{SiH}_2\text{M}$  ( $N = 1$  TO 6,  $M = 1$  TO 3) CLUSTERS**  
KATIRCIOGLU S., ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.177, sa.2, ss.373-378, 1993 (SCI-Expanded)
- CLXXV. **ELECTRONIC-ENERGY CALCULATION OF C-60 CLUSTERS**  
KATIRCIOGLU S., ERKOC S., HALICIOGLU T.  
MATERIALS CHEMISTRY AND PHYSICS, cilt.34, sa.1, ss.78-80, 1993 (SCI-Expanded)
- CLXXVI. **SIMULATION CALCULATIONS FOR GOLD CLUSTERS ON THE GAAS(110) SURFACE**  
ERKOC S., HALICIOGLU T., TILLER W.  
SURFACE SCIENCE, cilt.274, sa.3, ss.359-362, 1992 (SCI-Expanded)
- CLXXVII. **A NEW CLASS OF EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTIONS FOR BULK AND CLUSTER PROPERTIES**  
ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.171, sa.2, ss.317-324, 1992 (SCI-Expanded)
- CLXXVIII. **MOLECULAR-DYNAMICS COMPUTER-SIMULATION OF ALUMINUM CLUSTERS ( $\text{Al}_N$   $N = 3$  TO 55) - EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION CALCULATION**  
ELBAYYARI Z., ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.170, sa.1, ss.103-111, 1992 (SCI-Expanded)
- CLXXIX. **STRUCTURAL STABILITY AND ENERGETICS OF  $\text{Si}_4$  ISOMERS - TOTAL ELECTRONIC-ENERGY CALCULATION**  
KATIRCIOGLU S., ERKOC S.  
CHEMICAL PHYSICS LETTERS, cilt.184, ss.118-120, 1991 (SCI-Expanded)
- CLXXX. **STRUCTURAL STABILITY AND ENERGETICS OF AS, SB AND BI MICROCLUSTERS - EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION CALCULATION**  
KATIRCIOGLU S., ERKOC S.  
CHEMICAL PHYSICS LETTERS, cilt.182, sa.5, ss.451-454, 1991 (SCI-Expanded)
- CLXXXI. **STRUCTURAL STABILITY AND ENERGETICS OF SULFUR MICROCLUSTERS - AN MNDO CALCULATION**  
YILMAZ H., ERKOC S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.77, ss.63-76, 1991 (SCI-Expanded)
- CLXXXII. **STRUCTURAL STABILITY AND ENERGETICS OF C, SI, AND GE MICROCLUSTERS - EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION CALCULATION**  
ERKOC S.  
ZEITSCHRIFT FUR PHYSIK D-ATOMS MOLECULES AND CLUSTERS, cilt.19, ss.423-425, 1991 (SCI-Expanded)
- CLXXXIII. **EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION FOR SILVER AND GOLD - APPLICATION TO MICROCLUSTERS**  
ERKOC S.  
CHEMICAL PHYSICS LETTERS, cilt.173, sa.1, ss.57-62, 1990 (SCI-Expanded)
- CLXXXIV. **STRUCTURAL STABILITY AND ENERGETICS OF FCC METAL MICROCLUSTERS - EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION CALCULATION**  
ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.161, sa.1, ss.211-216, 1990 (SCI-Expanded)
- CLXXXV. **A NEW EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION - APPLICATION TO MICROCLUSTERS - ELEMENTS IN BCC, FCC, AND HCP STRUCTURES**  
ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.155, sa.2, ss.461-465, 1989 (SCI-Expanded)
- CLXXXVI. **A NEW EMPIRICAL MANY-BODY POTENTIAL-ENERGY FUNCTION - APPLICATION TO MICROCLUSTERS**  
ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.152, sa.2, ss.447-454, 1989 (SCI-Expanded)

- CLXXXVII. **MOLECULAR-DYNAMICS SIMULATION OF GALLIUM MICROCLUSTERS**  
KATIRCIOGLU S., ERKOC S.  
JOURNAL OF CRYSTAL GROWTH, cilt.94, sa.3, ss.807-809, 1989 (SCI-Expanded)
- LXXXVIII. **METALLIC PHASE OF AMORPHOUS-SILICON**  
ERKOC S., KATIRCIOGLU S.  
JOURNAL OF NON-CRYSTALLINE SOLIDS, cilt.107, ss.328-329, 1989 (SCI-Expanded)
- CLXXXIX. **DISSOCIATION OF Au-n (n=3,4) MICROCLUSTERS: A MOLECULAR DYNAMICS SIMULATION**  
Katircioglu S., Erkok S.  
MOLECULAR SIMULATION, cilt.4, sa.4, ss.247-250, 1989 (SCI-Expanded)
- CXC. **SELF-CONSISTENT FIELD CALCULATIONS FOR GAAS/GAALAS SAWTOOTH SUPERLATTICES**  
USLU B., ERKOC S.  
SOLID STATE COMMUNICATIONS, cilt.68, sa.2, ss.277-281, 1988 (SCI-Expanded)
- CXCI. **INTERATOMIC POTENTIALS WITH MULTI-BODY INTERACTIONS**  
HALICIOGLU T., PAMUK H., ERKOC S.  
PHYSICA STATUS SOLIDI B-BASIC RESEARCH, cilt.149, sa.1, ss.81-92, 1988 (SCI-Expanded)
- CXCII. **MOLECULAR-DYNAMICS SIMULATION OF GOLD MICROCLUSTERS**  
ERKOC S., KATIRCIOGLU S.  
CHEMICAL PHYSICS LETTERS, cilt.147, sa.5, ss.476-478, 1988 (SCI-Expanded)
- CXCIII. **SCATTERING OF HE FROM A CU(110) SURFACE**  
OZDER S., ERKOC S., ILTAN E.  
CHEMICAL PHYSICS LETTERS, cilt.135, sa.6, ss.582-586, 1987 (SCI-Expanded)

### **Diğer Dergilerde Yayınlanan Makaleler**

- I. **Two common terminological mistakes in scientific papers**  
ERKOÇ Ş.  
TURKISH JOURNAL OF PHYSICS, cilt.39, sa.3, ss.314-315, 2015 (ESCI)
- II. **Pre service Physics Teachers Comprehension of Quantum Mechanical Concepts**  
DİDİŞ KÖRHASAN N., ERYILMAZ A., ERKOÇ Ş.  
Eurasia Journal of Mathematics, Science & Technology Education, cilt.6, ss.227-235, 2010 (Hakemli Dergi)
- III. **Chapter 8 Thermal stability of carbon nanosystems: Molecular-dynamics simulations**  
Erkoç Ş., MALCIOĞLU O. B., TAŞCI E.  
Theoretical and Computational Chemistry, cilt.18, ss.201-226, 2007 (Scopus)

### **Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar**

- I. **Students Mental Models about the Quantization of Physical Observables**  
DİDİŞ KÖRHASAN N., ERYILMAZ A., ERKOÇ Ş.  
GIREP-MPTL 2014 International Conference, 7 - 12 Temmuz 2014
- II. **Increasing of H<sub>2</sub> storage in carbon nanotubes CNT(7,0), CNT(4,4), CNT(4,2) via doping with a boron nitride ring by molecular dynamics simulation studies**  
Onay A., ERKOÇ Ş.  
36th FEBS Congress of the Biochemistry for Tomorrows Medicine, Torino, İtalya, 25 - 30 Haziran 2011, cilt.278, ss.369
- III. **Oxygen-doped c-BN(110) surface: DFT calculations**  
KÖKTEN H., ERKOÇ Ş.  
11th Europhysical Conference on Defects in Insulating Materials (EURODIM), Pecs, Macaristan, 12 - 16 Temmuz 2010, cilt.15
- IV. **Titanium coverage on a single-wall carbon nanotube: Molecular dynamics simulations**

Oymak H., Erkoc S.

Conference of the NATO-Advanced-Study-Institute on Nanoengineered Nanofibrous Materials, Belek-Antalya, Türkiye, 1 - 12 Eylül 2003, cilt.169, ss.153-157

**V. Stability of carbon nanotori**

Yazgan E., Tasci E., Malcioglu O., Erkoc S.

Conference of the NATO-Advanced-Study-Institute on Nanoengineered Nanofibrous Materials, Belek-Antalya, Türkiye, 1 - 12 Eylül 2003, cilt.169, ss.241-244

## **Metrikler**

Yayın: 201

Atıf (WoS): 1843

Atıf (Scopus): 1767

H-İndeks (WoS): 23

H-İndeks (Scopus): 22