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Advising Theses

ERKOÇ Ş., Investigation of InP and SiGe nanomaterials via molecular dynamics simulations, Doctorate, N.NAYİR(Student), 2018

ERKOÇ Ş., Investigation of structural and electronic properties of ZnCdTe ternary alloy nanostructures, Doctorate, M.KURBAN(Student), 2016

ERKOÇ Ş., Structural Properties of ZnO Binary Alloy Nanosystems: Molecular-Dynamics Simulations, Doctorate, M.EMİN(Student), 2015

SEZGİ N. A., ERKOÇ Ş., Investigation of structural properties of boron carbide nanosystems under mechanical and thermal effects: Molecular dynamics simulations, Doctorate, Y.ŞİMŞEK(Student), 2014

Yazıcıoğlu Y., Erkoç Ş., Investigation of structural properties of metal nanorods: Molecular dynamics simulations, Postgraduate, H.YAĞLI(Student), 2014

ERKOÇ Ş., Structural, electronic and magnetic properties of various nanosystems : molecular dynamics simulations and density functional theory calculations, Doctorate, A.Sholejh(Student), 2014

ERKOÇ Ş., Structural,electronic and magnetic properties of various nanosystems:n Molecular dynamics simulations and density functional theory calcualtions, Doctorate, S.SALAEI(Student), 2014

ERKOÇ Ş., Structural, electronic, and magnetic properties of smmcon ($m + n - 3$) microclusters: density functional theory calculations, Postgraduate, N.Kara(Student), 2013

ERKOÇ Ş., Structural, electronic, and magnetic properties of SmMCoN ($M+N < 3$)microclusters: Density functioinal theory calculations, Postgraduate, N.KARA(Student), 2013

ERKOÇ Ş., Investigation of the structural properties of low dimensional nanostructures: Molecular dynamics simulations, Postgraduate, B.ÖZDAMAR(Student), 2013

AYDINOL M. K., ERKOÇ Ş., Investigation of the structural properties of silicene nanoribbons by molecular dynamics simulations, Postgraduate, A.İNCE(Student), 2012

ERKOÇ Ş., Acceleration of molecular dynamics simulation for TERSOFF2 potential through reconfigurable hardware, Postgraduate, B.VARGÜN(Student), 2012

GÜVENÇ YAZICIÖGLU A., ERKOÇ Ş., Structural properties of defected graphene nanoribbons under tension: Molecular-dynamics simulations, Postgraduate, B.TÜZÜN(Student), 2012

ERYILMAZ A., ERKOÇ Ş., Investigation of undergraduate students' mental models about the quantization of physical observables, Doctorate, D.NİLÜFER(Student), 2012

ÖNAL I., ERKOÇ Ş., Quantum mechanical treatment of fullerene-based systems doped with various metal and non-metal elements as prospective spin-qubits, Postgraduate, S.POLAD(Student), 2010

ERKOÇ Ş., Investigation of biologically important small molecules: quantum chemical and molecular dynamics calculations, Doctorate, E.Deniz(Student), 2010

ERKOÇ Ş., Quantum monte carlo methods for fermionic systems: Beyond the fixed-node approximation, Doctorate, N.DUGAN(Student), 2010

ERKOÇ Ş., Tailoring one dimensional novel nano structures for specific applications using tools of molecular modeling, Doctorate, O.BARIŞ(Student), 2008

ERKOÇ Ş., Hydrogen storage capacity of nanosystems: molecular dynamics simulations, Postgraduate, A.Koyuncular(Student), 2008

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

ERKOÇ Ş., Hydrogen storage capacity of nanosystems: Molecular -dynamics simulations, Postgraduate, A.KOYUNCULAR(Student), 2008

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

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

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

ERKOÇ Ş., Theoretical investigaton of AltıNi ternary glusters : density functioanal theory calculations and molecular dynamics simulations, Doctorate, H.Oymak(Student), 2004

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

ERKOÇ Ş., Stability of carbon nanotubes and nanorods under heat theatment : Molecular dynamics simulations, Postgraduate, O.Barış(Student), 2003

ERKOÇ Ş., Simulation of the casimir effect for various geometries., Postgraduate, E.TAŞCI(Student), 2002

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

ERKOÇ Ş., Simulation of condenser microphone behavior, Postgraduate, C.KIRBAŞ(Student), 1999

ERKOÇ Ş., Molecular dynamics simulation of water clusters, Postgraduate, E.GÜNEYLER(Student), 1999

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

ERKOÇ Ş., Geometry optimization of small copper clusters: Monte Carlo simulations study., Postgraduate, S.Riad(Student), 1998

ERKOÇ Ş., Molecular-dynamics computer simulation of copper clusters:structural stability, energetics, and melting, Postgraduate, C.Özdogan(Student), 1996

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

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

ERKOÇ Ş., Structural stability and energetics of carbon clusters:Tersoff empirical many-body potential energy function calculation, Postgraduate, M.TÜRELİ(VIDAL)(Student), 1993

ERKOÇ Ş., Structural stability and energetics of carbon clusters:Tersoff emprirical many-body potential energy functon calculation, Postgraduate, M.Türel(Vidal)(Student), 1993

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

ERKOÇ Ş., Structural stability and energetics of P, S, and C microclusters, Postgraduate, Y.TAHTAMONİ(Student), 1990

ERKOÇ Ş., Structural stability and energetics of selenium and tellurium microclusters:empirical many-body potential energy function calculation, Postgraduate, A.ÜNLÜ(Student), 1990

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

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

Published journal articles indexed by SCI, SSCI, and AHCI

- 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, vol.123, no.19, pp.4303-4313, 2019 (SCI-Expanded)
- II. **Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its**

Application to GeO₂/Ge Interfaces

Nayir N., van Duin A. C. T., ERKOÇ Ş.

JOURNAL OF PHYSICAL CHEMISTRY C, vol.123, no.2, pp.1208-1218, 2019 (SCI-Expanded)

- III. **A density functional theory study on the structural and electronic properties of Pb_xSb_ySe_z (x plus y plus z=2, 3) clusters**

Pekoz R., ERKOÇ Ş.

INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.32, no.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, vol.88, pp.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, vol.122, pp.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, vol.16, no.2, pp.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, vol.464, pp.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, vol.37, no.1, 2016 (SCI-Expanded)

- IX. **Structural properties of indium phosphide nanorods: molecular dynamics simulations**

Nayir N., TAŞCI E., ERKOÇ Ş.

INTERNATIONAL JOURNAL OF NANOTECHNOLOGY, vol.13, pp.809-831, 2016 (SCI-Expanded)

- X. **Structural and Electronic Properties of ZnmCdn,Te-k (m plus n plus k=2-4) Clusters: DFT Calculations**

Kurban M., ERKOÇ Ş.

JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.12, no.9, pp.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, vol.12, no.9, pp.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, vol.12, no.9, pp.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, vol.12, no.6, pp.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, vol.12, no.3, pp.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, vol.23, no.6, pp.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, vol.10, no.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, vol.14, no.1, pp.57-67, 2014 (SCI-Expanded)
- XVIII. **Structural Properties of beta-Fe2O3 Nanorods Under Strain: Molecular Dynamics Simulations**
Alaei S., ERKOÇ Ş.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.11, no.1, pp.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, vol.79, pp.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, vol.13, no.10, pp.6597-6610, 2013 (SCI-Expanded)
- XXI. **Structural Properties of ZnO Nanoparticels and Nanorings: Molecular Dynamics Simulations**
Kilic M. E., ERKOÇ Ş.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.10, no.6, pp.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, vol.10, no.2, pp.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, vol.10, no.1, pp.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, vol.10, no.1, pp.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, vol.10, no.1, pp.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, vol.26, no.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, vol.249, no.1, pp.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, vol.44, no.1, pp.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, vol.50, no.10, pp.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, vol.8, no.4, pp.694-706, 2011 (SCI-Expanded)

- XXXI. **Silicene nanoribbons: Molecular-dynamics simulations**

Ince A., ERKOÇ Ş.

COMPUTATIONAL MATERIALS SCIENCE, vol.50, no.3, pp.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, vol.7, no.10, pp.1889-1893, 2010 (SCI-Expanded)

- XXXIII. **Quantum chemical treatment of beta-sitosterol molecule**

Kurban S., ERKOÇ F., ERKOÇ Ş.

PHARMACEUTICAL BIOLOGY, vol.48, no.6, pp.637-642, 2010 (SCI-Expanded)

- XXXIV. **Density Functional Theory Calculations on Polyacene Molecules**

Pekoz R., ERKOÇ Ş.

ADVANCED SCIENCE LETTERS, vol.3, no.1, pp.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, vol.114, no.4, pp.1897-1905, 2010 (SCI-Expanded)

- XXXVI. **Quantum chemical investigation of nitrotyrosine (3-nitro-L-tyrosine) and 8-nitroguanine**

ERKOÇ Ş., ERKOÇ F., SEPİCİ DİNCEL A.

AMINO ACIDS, vol.38, no.1, pp.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, vol.36, no.10, pp.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, vol.404, pp.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, vol.42, no.2, pp.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, vol.111, no.10, pp.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, vol.46, no.4, pp.821-827, 2009 (SCI-Expanded)

- XLII. **Structural and thermochemical properties, and energetics of C-8(NO₂)₈ and C-20(NO₂)_{4n} (n=0-4)**

Pekoz R., ERKOÇ Ş.

COMPUTATIONAL MATERIALS SCIENCE, vol.46, no.4, pp.849-853, 2009 (SCI-Expanded)

- XLIII. **A density functional theory study on the structures and energetics of CdmTen clusters (m + n <= 6)**

Pekoz R., ERKOÇ Ş.

COMPUTATIONAL MATERIALS SCIENCE, vol.45, no.4, pp.912-920, 2009 (SCI-Expanded)

- XLIV. **Molecular Mechanics and Molecular Dynamics Simulations of Carbon Based Nanogears**

- Tascı E., ERKOÇ Ş.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.6, no.4, pp.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, vol.6, no.4, pp.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, vol.6, no.4, pp.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, vol.6, no.4, pp.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, vol.6, no.4, pp.933-941, 2009 (SCI-Expanded)
- XLIX. **A Special Issue on Physics and Chemistry of Nanoparticles**
Erkoc S.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.6, no.4, pp.805, 2009 (SCI-Expanded)
- L. **Genetic algorithm-Monte Carlo hybrid geometry optimization method for atomic clusters**
Dugan N., ERKOÇ Ş.
COMPUTATIONAL MATERIALS SCIENCE, vol.45, no.1, pp.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, vol.6, no.1, pp.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, vol.24, no.3, pp.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, vol.40, no.9, pp.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, vol.4, no.1, pp.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, vol.40, no.8, pp.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, vol.245, no.4, pp.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, vol.8, no.2, pp.469-478, 2008 (SCI-Expanded)
- LVIII. **Li+ and Li interactions with carbon nanocage structures**
Pekoez R., ERKOÇ Ş.
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, vol.8, no.2, pp.675-678, 2008 (SCI-Expanded)
- LIX. **Structural properties and stability of nanoclusters**
Ustuenel H., Erkoc S.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.4, no.5, pp.928-956, 2007 (SCI-Expanded)

- LX. **Structural and electronic properties of defected carbon nanocapsules**
Pekoz R., Erkoc S.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.4, no.4, pp.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, vol.7, pp.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, vol.28, no.2, pp.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, vol.36, no.2, pp.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, vol.18, pp.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, vol.22, pp.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.
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- LXVII. **Density functional theory calculations for [C₂H₄N₂O₆]((n)) (n=0,+1,-1)**
Turker L., Erkoc S.
JOURNAL OF HAZARDOUS MATERIALS, vol.136, no.2, pp.164-169, 2006 (SCI-Expanded)
- LXVIII. **Structural and electronic properties of dipropyl sulfide: A theoretical investigation**
Calisir E. D., Erkoc S.
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- LXIX. **Structural properties of copper nanoparticles: Modified diffusion Monte Carlo simulations**
Dugan N., Erkoc S.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.17, no.8, pp.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, vol.426, pp.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, vol.104, pp.2027-2036, 2006 (SCI-Expanded)
- LXXII. **Structural and electronic properties of the DPPC molecule**
Erkoc S., Korkmaz F.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.17, no.7, pp.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, vol.17, no.6, pp.795-803, 2006 (SCI-Expanded)
- LXXIV. **Structural and electronic properties of bamboo-like carbon nanostructure**
Erkoc S.
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- LXXV. **Metal atom endohedrally doped C-20 cage structure: (X@C-20; X = Ni, Fe, Co)**
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