Prof. ŞAKİR ERKOÇ

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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 nanosytems:n Molecular dynamics simulations and density functional theory calcualtions, Doctorate, S.ALAEI(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 functoinal 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 YAZICIOĞLU 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 AltiNi 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
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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
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ERKOÇ Ş., Molecular-dynamics computer simulation of copper clusters:structural stability, energetics, and melting, Postgraduate, C.Özdoğan(Student), 1996
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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(VİDAL)(Student), 1993
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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.
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Nayir N., van Duin A. C. T., ERKOÇ Ş.
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III. **A density functional theory study on the structural and electronic properties of PbxSbySez (x plus y plus z=2, 3) clusters**
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IV. **Segregation formation, thermal and electronic properties of ternary cubic CdZnTe clusters: MD simulations and DFT calculations**
KURBAN M., ERKOÇ Ş.
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V. **Mechanical properties of CdZnTe nanowires under uniaxial stretching and compression: A molecular dynamics simulation study**
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VI. **Structural Properties of Pristine and Defected ZnO Nanosheets Under Biaxial Strain: Molecular Dynamics Simulations**
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VII. **Structural and thermal properties of Cd-Zn-Te ternary nanoparticles: Molecular-dynamics simulations**
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IX. **Structural properties of indium phosphide nanorods: molecular dynamics simulations**
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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**
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XIII. **Carbon Nanobuggy is Ready for a Test Drive!**
Tasci E. S., ERKOÇ Ş.
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XIV. **X-Doped (X = C, N, F, P) ZnO Sheet: Density Functional Theory Calculations**
KÖKTEN H., ERKOÇ Ş.

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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**
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XIX. **Evolution of the electronic structure and properties of charged titanium doped aluminum nanoclusters**
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JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.10, no.2, pp.470-480, 2013 (SCI-Expanded)

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XXIV. **Molecular Dynamics Simulations of Zinc Oxide Nanostructures Under Strain: I-Nanoribbons**
Kilic M. E., ERKOÇ Ş.
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XXV. **Molecular Dynamics Simulations of ZnO Nanostructures Under Strain: II-Nanorods**
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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-)**
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Ince A., ERKOÇ Ş.
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XXVIII. **Energetics and structural properties of carbon and oxygen doped hexagonal boron nitride sheets**
KÖKTEN H., ERKOÇ Ş.
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XXIX. **Structural properties of boron carbide nanoparticles: Application of a new set of Stillinger-Weber**

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COMPUTATIONAL MATERIALS SCIENCE, vol.50, no.10, pp.2950-2954, 2011 (SCI-Expanded)

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Polad S., ERKOÇ Ş.
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XXXII. **Effects of Water Related Defects on Pentacene and Picene Molecules**
Pekoz R., ERKOÇ Ş.
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XXXVI. **Quantum chemical investigation of nitrotyrosine (3-nitro-L-tyrosine) and 8-nitroguanine**
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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**
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PHYSICA B-CONDENSED MATTER, vol.404, pp.4937-4938, 2009 (SCI-Expanded)

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XL. **Quantum-chemical treatment of the linoleic acid molecule and two of its conjugated isomers**
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XLI. **Analyzing Fe-Zn system using molecular dynamics, evolutionary neural nets and multi-objective genetic algorithms**
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XLII. **Structural and thermochemical properties, and energetics of C-8(NO2)(8) and C-20(NO2)(4n) (n=0-4)**
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Tasci E., ERKOÇ Ş.
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XLV. **Structural and Electronic Properties of GamSen Microclusters: Density Functional Theory Calculations**
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L. **Genetic algorithm-Monte Carlo hybrid geometry optimization method for atomic clusters**
Dugan N., ERKOÇ Ş.
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LI. **Endohedral Li/Li+ Doped Stone-Wales Defected Carbon Nanocapsules**
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LX. **Structural and electronic properties of defected carbon nanocapsules**
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