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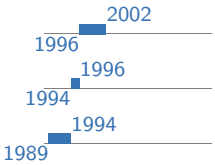
Cem Özdoğan

Curriculum Vitæ

Education



Ph.D. in Physics, *Middle East Technical University*, Ankara Turkey.

M.Sc. in Physics, *Middle East Technical University*, Ankara Turkey.

B.Sc. in Physics, *Middle East Technical University*, Ankara Turkey.

PhD thesis

title *Order(N) Parallel Tight Binding Molecular Dynamics Computer Simulation: Application to Carbon Nanotubes*

supervisors Prof. Dr. Gülay Dereli

description An O(N) Parallel Tight–Binding Molecular Dynamics (TBMD) algorithm in the simulations of Single Wall Carbon Nanotubes (SWCNT) is developed. We have applied O(N) (Divide and Conquer scheme) technique in Carbon nanotube simulation and parallelized our O(N) TBMD program. The structural stability and energetics of 10x10 and 17x0 tubes are investigated. Elastic properties under uniaxial strain are studied at room temperature. The Young's modulus, tensile strength, Poisson ratio and frequency of vibrations are calculated. We have observed disintegrations under large strains.

Master thesis

title *Molecular Dynamics Computer Simulation of Copper Clusters: Structural Stability, Energetics and Melting*

supervisors Prof. Dr. Şakir Erkoç

description We have investigated cluster properties of copper using our developed Molecular–Dynamics code. In the simulation an empirical potential energy function (PEF) proposed by Erkoç has been used, which contains two–body atomic interactions. The structural stability and energetics of Cu_n $(n = 13 - 135)$ shell like structured clusters have been investigated at temperatures $T = 1\ K$ and $T = 300\ K$. The melting behavior of clusters $n = 13$ and $n = 55$ have been investigated.

Languages

Turkish	Native	*Mother Tongue*
English	Fluent	*Daily Practice*

Interests

Physics

- Atomic and Molecular [10] Clusters [7–9, 11, 16, 17, 21, 22, 24, 25, 32–34, 40, 41]
- Classical and Quantum Molecular Dynamics Simulations [3, 4, 7, 8, 20, 23, 26–30, 32, 33, 42, 43, 45, 47]
- Many Body Potentials [30, 47]
- Ion-surface Collisions [20, 26, 42, 43]
- Hydrogen Storage [21, 22, 24]
- Energy Storage - Supercapacitors [2]

Chemistry Electronic Structure Calculations/Computational Chemistry [1–6, 9–11, 13, 15–19, 21, 22, 24, 25, 31, 34, 40, 41, 46]

Computer Parallel Computing & High Performance Computing (HPC) [7, 8, 12, 14, 20, 23, 26–29, 32, 33, 35, 36, 42–46], Data Mining [12, 14, 35, 36, 44]

Main Focus Carbon [1–6, 13, 15, 18, 19, 23, 27, 28, 31, 38, 41, 45, 46] and boron [1–5, 9, 11, 16, 17, 25, 29, 31, 34, 40] based nano and periodic systems: Structural, electronic and magnetic properties

Computer and Scientific Skills

Development, Software and Technical

EAM MD Parallelization of an Embedded Atom Model Molecular Dynamics (EAM MD) program and application to ion-surface collisions and clusters [7, 8, 20, 26, 32, 33, 42, 43]

TBMD Writing and Parallelization of a Tight Binding Molecular Dynamics (TBMD) program and application to carbon nanotubes [23, 27–29, 45]

MD Writing of a Classical Molecular Dynamics (MD) program and application to copper clusters [30, 47]

Languages Fortran, C, C++, Bash Scripts, Python

Compilers Intel, Portland

Debuggers TotalView, gdb

Libraries (Sca)+Lapack, Blas, MPI(Message Passing Interface), PVM (Parallel Virtual Machine), OpenMP

General LaTeX, PovRay

Math Matlab, Mathematica

Networking LAN (Local Area Network) administration with Linux

Cluster Build-up, Administration

Technical Course CISCO CCNA Computer Networks, October 2006-June 2007, Ankara, METU Türkiye (Certificate)

Technical Course Joint ICTP-INFM School on High Performance Computing on Linux Clusters, 31 January-15 February 2002, Trieste, Italy (Participation)

Technical Course Performance Optimization and Parallelization on Sun Systems, Istanbul, Turkey April 4-6, 2000 (Participation)

Computational Chemistry/Physics

Packages VASP, Gaussian, QuantumATK, (Tran)siesta

Visualization XCrysDen, Chemcraft, Gaussview, QuantumATK (VNL)

Experience

Coordination

2012–2015 **Physics Courses**, *Cankaya University*, General Coordinator, University Wide.

2011–2014 **Course Timetabling**, *Cankaya University*, General Coordinator, University Wide.

2008–2010 **Erasmus**, *Cankaya University*, Coordinator, Computer Engineering Department.

2002–2015 **Parallel and Scientific Computation Cluster**, *Cankaya University*, Administration, University Wide.

2010–2010 **New Trends in Nanotechnology and Nonlinear Dynamical Systems** , *Cankaya University*, Scientific and Organizing Committee, Symposium.

2008–2008 **International Workshop on New Trends in Science and Technology**, *Cankaya University*, Scientific and Organizing Committee, Symposium.

Short Visits

2010–2010 **Visiting Scientist**, *Prof. Dr. Ravindra Pandey*, Michigan Technological University, USA, 6 weeks.

Transport properties of azobenzene; Transiesta

2009–2009 **Visiting Scientist**, *Prof. Dr. Alexander Quandt*, University of Greifswald, Germany, 2 weeks.

Simulation of novel graphene based nanosized materials; Vasp

2008–2008 **Researcher**, *Prof. Dr. Alexander Quandt*, University of Greifswald, Germany, 2 weeks.

Simulation of novel graphene based nanosized materials; Vasp

2007–2007 **Researcher**, *Prof. Dr. Alexander Quandt*, University of Greifswald and HLRS Stuttgart, Germany, 10 weeks.

An ab initio study of planar boron-carbon interfaces; Vasp

Project Activities

2017–2021 **Supervisory**, *Design of Planar and Tubular Nanostructured Hetero Double Layer Electrostatic Supercapacitors and Investigation of Energy Storage Capabilities with First Principle Methods*, TÜBİTAK, MFAG 115F137.

Scientific Research Project supported by The Scientific and Technical Research Council of Turkey

2015–2018 **Researcher**, *Investigation of the structural, electronic, and magnetic properties of hexagonal boron nitride/graphene (h-BN/G) in-plane hybrid and hetero structures, and design of nanosystems functionalized with defects*, TÜBİTAK, MFAG 114F426.

Scientific Research Project supported by The Scientific and Technical Research Council of Turkey

2007–2007 **Supervisory**, *An ab initio study of planar boron-carbon interfaces*, HPC-EUROPA, RII3-CT-2003-506079.
Research Infrastructure Action under the FP6 "Structuring the European Research Area" Programme

2005–2007 **Researcher**, *Storage of Hydrogen as Clean Energy Resource on Nanostructures*, TÜBİTAK, TBAG (105T084).
Scientific Research Project supported by The Scientific and Technical Research Council of Turkey

2000–2001 **Researcher**, *Computer Simulation of Electronic Structure of Nanotubes and Effects of the Stress and Topological Defects on the Electronic Structure*, TÜBİTAK, TBAG (199T106).
Scientific Research Project supported by The Scientific and Technical Research Council of Turkey

2000–2002 **Researcher**, *Order(N) Parallel Computer Simulation of Electronic Structure of Nanotubes*, METU, AFP-2000-07-02-11.
Scientific Research Project supported by Middle East Technical University

Supervising

2017–2021 **PhD**, *Habibu Aminu Hussain, Izmir Katip Celebi University*, A First Principle Investigation of the Effect of Vacancies on Structural, Electronic and Magnetic Properties of Graphene and h-BN Hybrid, Supervisor.
Completed

2014–2020 **PhD**, *Nazan Kara, Middle East Technical University*, Carbon Based Nano-Structure Supercapacitors for Energy Storage, Co-supervisor.
Not Completed

2010–2011 **MSc**, *Ahmet Artu Yıldırım, Cankaya University*, Parallelization Study on the Clustering Technique to Mine Large Datasets, Supervisor.
Completed

2009–2010 **MSc**, *Afşar Türk, Cankaya University*, Heating Effect of Electromagnetıc Fields on Human Head at GSM Frequencies, Co-supervisor.
Completed

2004–2005 **MSc**, *Hüseyin Şahin Akbal, Cankaya University*, Developing Tools For The Enhancement of Remote Sensing Images and Parallel Programming Applications, Supervisor.
Completed

Academics

2019– **Professor**, *Department of Engineering Sciences, İzmir Kâtip Çelebi University*, İzmir.

- Teaching.
  - Physics I;
  - Physics II;
  - Scientific Computing with Python;
  - Introduction to High Performance and Parallel Computing.

2017–2018 **Professor**, *Department of Engineering Sciences, İzmir Kâtip Çelebi University*, İzmir, Chairman.

- Teaching.
  - Physics I;
  - Physics II;
  - Engineering Quantum Mechanics.

2016–2017 **Associate Professor**, *Department of Engineering Sciences, İzmir Kâtip Çelebi University*, İzmir.

- Teaching.
  - Physics II;
  - Engineering Quantum Mechanics;
  - Electrical, Optical and Magnetic Proprties of Materials.

2013–2015 **Associate Professor**, *Department of Materials Science and Engineering, Çankaya University*, Ankara, Chairman.

- Teaching.
  - Materials Science and Engineering Orientation;
  - Numerical Methods;
  - Parallel Computing;
  - Physics I;
  - Physics II.
- Technical & Coordination.
  - Administration and maintenance Parallel and Scientific Computation Cluster;
  - Administration and maintenance Teaching Purpose Cluster;
  - Coordinator of Course Timetabling: University wide;
  - General Coordinator of Physics I and Physics II Courses: University wide.

2011–2013 **Associate Professor**, *Department of Materials Science and Engineering, Çankaya University*, Ankara, Founder Acting Chairman.

- Teaching.
  - General Physics for Engineering I;
  - Parallel Computation (Graduate);
  - Numerical Computation;
  - Operating Systems;
  - Parallel Computing;
  - Physics II;
  - Statistical Computations.
- Technical & Coordination.
  - Administration and maintenance Parallel and Scientific Computation Cluster;
  - Administration and maintenance Teaching Purpose Cluster;
  - Coordinator of Course Timetabling: University wide;
  - General Coordinator of Physics I and Physics II Courses: University wide.

2009–2011 **Associate Professor**, *Department of Computer Engineering, Çankaya University*, Ankara, Vice Chairman.

2009–2009 **Associate Professor (Condensed Matter Physics; Computational Sciences)**, *Department of Computer Engineering, Çankaya University*, Ankara.

2002–2009 **Assistant Professor**, *Department of Computer Engineering, Çankaya University*, Ankara.

- Teaching.
  - Numerical Computation;
  - Operating Systems;
  - Parallel Computing;
  - Parallel Computation (Graduate);
  - Statistical Computations;
  - Systems Programming.
- Technical.
  - Administration and maintenance Parallel and Scientific Computation Cluster;
  - Administration and maintenance Teaching Purpose Cluster.

2001–2002 **Instructor**, *Department of Computer Engineering, Çankaya University*, Ankara.

- Teaching.
  - Advanced Programming Languages (Delphi);
  - Computer Literacy;
  - Introduction to Computers and Programming, Programming in C;
  - Object Oriented Programming, Programming in C++.
- Technical.
  - Building up Parallel and Scientific Computation Cluster http://siber.cankaya.edu.tr/boron-ganglia/ (NFS, PBS);
  - Building up Teaching Purpose Cluster for CENG471 & CENG505 Parallel Computing Courses http://wee.cankaya.edu.tr/ganglia/ (Diskless booting, NFS (Network File System), PBS (Portable Batch System)).

1999–2001 **Research Assistant**, *Department of Physics, Middle East Technical University*, Ankara.

- Assisting.
  - Building up Parallel and Scientific Computation Cluster;
  - Elementary Condensed Matter Physics, Recitation;
  - General Physics I & II, Laboratory & Recitation.

1994–1999 **Research Assistant**, *Department of Physics, Kırıkkale University*, Ankara.

- Assisting.
  - Building, maintenance and administrate the servers;
  - General Physics I & II, Laboratory & Recitation.

Vocational

1993–1993 **Technical Person**, *Department of Biophysics, Hacettepe University*, Ankara.

Did technical work. During 8 months in a project supported by TÜBİTAK (The Scientific and Technical Research Council of Turkey), in a position to assist for computer and electronics related works.

Editorial

2013–2014 **The Scientific World Journal**, *Hindawi Publishing Corporation*, SCI-Expanded, Editorial Board: Atomic and Molecular Physics.

2012–2012 **Turkish Journal of Electrical Engineering and Computer Sciences**, *TÜBITAK*, SCI-Expanded, Assistant Editor.

Panelist

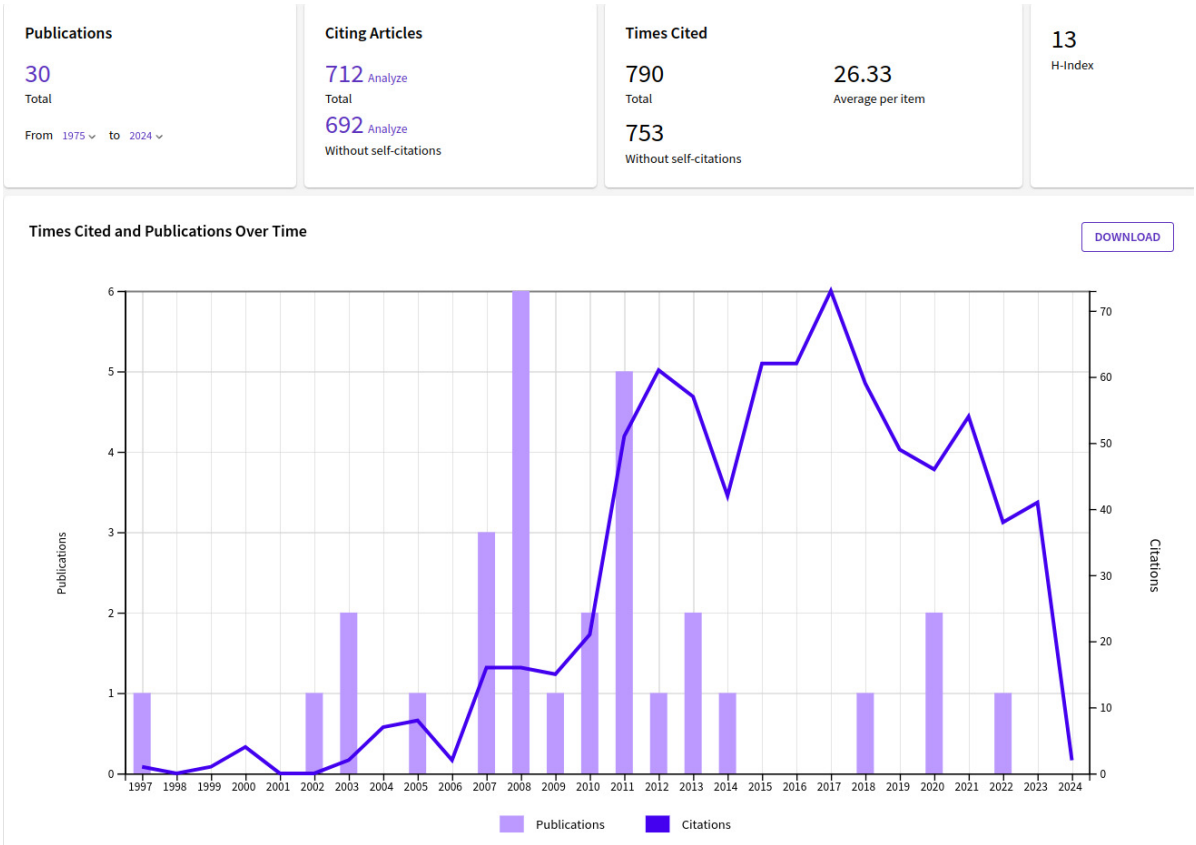
2012– **Panelist and External Reviewer**, *MFAG/MAG of*, TÜBİTAK, The Scientific and Technical Research Council of Turkey.

Reviewer

- Computational Materials Science - 1
- Diamond and Related Materials - 1
- Journal of Inorganic and Organometallic Polymers and Materials - 1
- Journal of Physical Chemistry C - 1
- Molecular Simulation - 1
- Physical Review A - 1
- Physcial Review B - 5
- RSC Advances - 10
- RSC Journal of Materials Chemistry A - 1
- RSC New Journal of Chemistry - 1
- RSC Physical Chemistry Chemical Physics - 1
- Turkish Journal of Electrical Engineering and Computer Sciences - 2
- Turkish Journal of Chemistry - 1
- Turkish Journal of Physics - 4
- Cankaya University Journal of Science and Engineering - 1

Citations

- Web of Science Citations at February 10, 2024



- Google Scholar Citations at February 10, 2024

	All	Since 2019
Citations	1169	321
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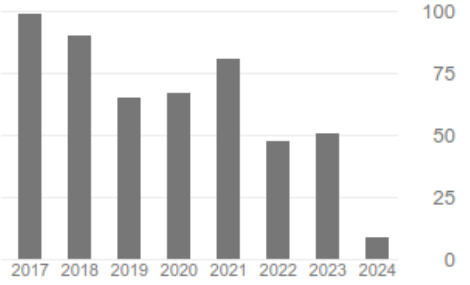
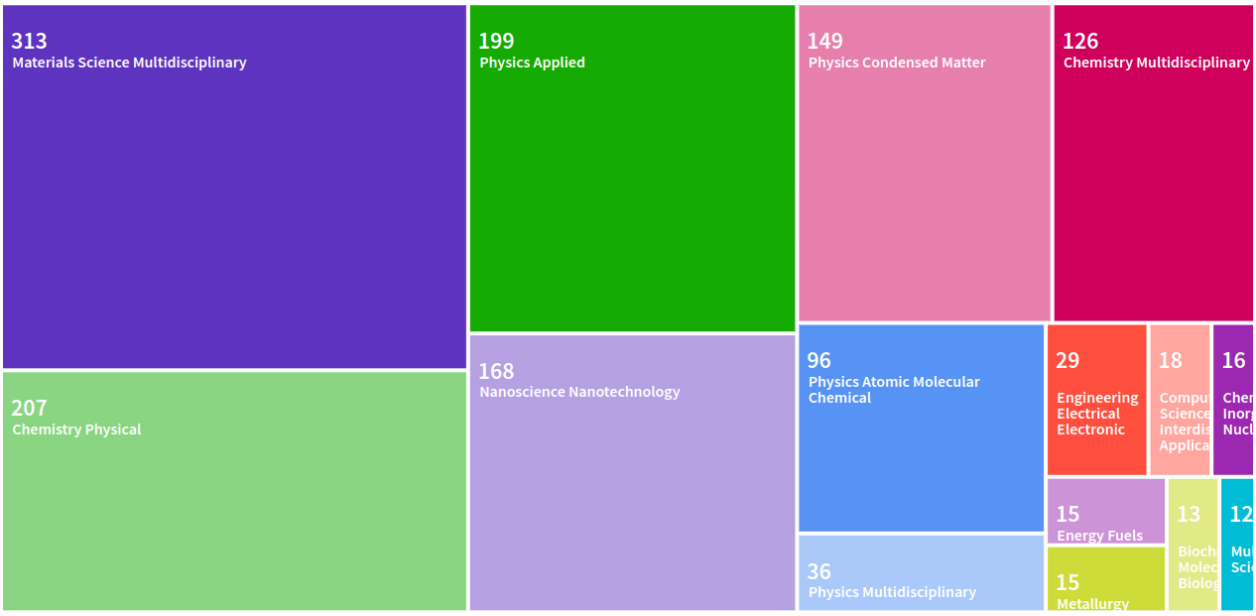


- TÜBİTAK Rating of Publications

Journal	ISSN	Article Influence Score	Year	# of Publications
MATERIALS SCIENCE AND ENGINEERING B-ADVANCED FUNCTIONAL SOLID-STATE MATERIALS	0921-5107	0.544	2023	1
FLATCHEM	2452-2627	0.854	2022	1
SOLID STATE SCIENCES	1293-2558	0.356	2019	1
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS	0304-8853	0.466	2019	1
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS	0022-3697	0.371	2019	1
PHILOSOPHICAL MAGAZINE	1478-6435	0.515	2020	1
JOURNAL OF PHYSICAL CHEMISTRY C	1932-7447	1.017	2020	2
MATERIALS TRANSACTIONS	1345-9678	30,200	2018	1
PHYSICAL REVIEW B	2469-9950	1.089	2020	5
JOURNAL OF CHEMICAL CRYSTALLOGRAPHY	1074-1542	4,440	2018	1
JOURNAL OF PARALLEL AND DISTRIBUTED COMPUTING	0743-7315	0.542	2020	1
Procedia Computer Science	1877-0509			1
COMMUNICATIONS IN NONLINEAR SCIENCE AND NUMERICAL SIMULATION	1007-5704	0.885	2020	1
CHINESE JOURNAL OF CHEMICAL PHYSICS	1674-0068	4,150	2018	1
PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS	0370-1972	0.412	2019	1
NANOTECHNOLOGY	0957-4484	0.744	2019	2
MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING	0965-0393	0.785	2020	1
PHYSICA SCRIPTA	0031-8949	0.385	2019	1
ICTON Mediterranean Winter Conference	978-1-4244-3484-8			1
Romanian Journal of Information Science and Technology	1453-8245	8.630	2018	1
JOURNAL OF MOLECULAR STRUCTURE	0022-2860	0.262	2019	1
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	0020-7608	0.730	2020	1
INTERNATIONAL JOURNAL OF MODERN PHYSICS C	0129-1831	9.100	2018	1
COMPUTER PHYSICS COMMUNICATIONS	0010-4655	1.625	2020	1
Zeitschrift fur Physik D-Atoms Molecules and Clusters	0178-7683			1
				31

- Web of Science Categories



Journal Publications (Web of Science)

2023

[1] Nurten Akman and Cem Özdoğan. "Modulation of electronic and magnetic properties of graphene-triangular h-BN hybrid through monovacancy: Carbon vacancy-BN size coupling". In: *Materials Science and Engineering: B* 298 (2023), 116863 (Cited 0 time). DOI: https://doi.org/10.1016/j.mseb.2023.116863.

2022

[2] Cem Özdoğan and Hatice Kökten. "An approach for quantum capacitance of graphene, carbon nanotube, silicene and hexagonal boron nitride nanoscale supercapacitors by non-equilibrium Green's function method". In: *FlatChem* 31 (2022), 100313 (Cited 1 time). DOI: https://doi.org/10.1016/j.flatc.2021.100313.

2020

[3] Habibu Aminu Hussain, Nurten Akman, and Cem Özdoğan. "Investigation of the mono vacancy effects on the structural, electronic and magnetic properties of graphene hexagonal-boron nitride in-plane hybrid embracing diamond shaped graphene island". In: *Solid State Sciences* 108 (2020), 106395 (Cited 2 time). DOI: https://doi.org/10.1016/j.solidstatesciences.2020.106395.

2020

[4] Nurten Akman and Cem Özdoğan. "Vacancy induced robust magnetism in graphene hexagonal-boron nitride in-plane hybrids with hexagonal shaped islands". In: *Journal of Magnetism and Magnetic Materials* 502 (2020), 166530 (Cited 4 times). DOI: 10.1016/j.jmmm.2020.166530.

2018

[5] Nurten Akman and Cem Özdoğan. "Island shape, size and interface dependency on electronic and magnetic properties of graphene hexagonal-boron nitride (h-BN) in-plane hybrids". In: *Journal of Physics and Chemistry of Solids* 115 (2018), 187–198 (Cited 10 times). DOI: 10.1016/j.jpcs.2017.12.025.

2014

[6] Cem Özdoğan, Jens Kunstmann, and Alexander Quandt. "Localization of metallicity and magnetic properties of graphene and of graphene nanoribbons doped with boron clusters". In: *Philosophical Magazine* 94.16 (2014), 1841–1858 (Cited 8 times). DOI: 10.1080/14786435.2014.895875.

2013

[7] Hani A. Alarifi, Murat Atiş, Cem Özdoğan, Amming Hu, Mustafa Yavuz, and Y. Zhou. "Determination of Complete Melting and Surface Premelting Points of Silver Nanoparticles by Molecular Dynamics Simulation". English. In: *Journal of Physical Chemistry C* 117.23 (June 2013), 12289–12298 (Cited 96 times). DOI: 10.1021/jp311541c.

2013

[8] Hani A. Alarifi, Murat Atiş, Cem Özdoğan, Amming Hu, Mustafa Yavuz, and Y. Zhou. "Molecular Dynamics Simulation of Sintering and Surface Premelting of Silver Nanoparticles". English. In: *Materials Transactions* 54.6 (June 2013), 884–889 (Cited 43 times). DOI: 10.2320/matertrans.MD201225.

2012

[9] Murat Taş, Nurten Akman, Cem Özdoğan, and Ihsan Boustani. "Fragmentation and Coulomb explosion of multicharged small boron clusters". English. In: *Physical Review B* 85.23 (June 2012), 235445 (Cited 1 time). DOI: 10.1103/PhysRevB.85.235445.

2011

[10] Çiğdem Yuksektepe, Canan Kazak, Cem Özdoğan, Ziya Burhanettin Guvenc, Orhan Büyükgüngör, Figen Arslan, and Mustafa Odabaşoğlu. "Synthesis, Molecular Structure and DFT Study of 2-(N-Benzoylbenzamido)pyridine-3-yl benzoate". English. In: *Journal of Chemical Crystallography* 41.10 (Oct. 2011), 1520–1527 (Cited 0 time). DOI: 10.1007/s10870-011-0134-3.

2011

[11] Nurten Akman, Murat Taş, Cem Özdoğan, and Ihsan Boustani. "Ionization energies, Coulomb explosion, fragmentation, geometric, and electronic structures of multicharged boron clusters B-n (n=2-13)". English. In: *Physical Review B* 84.7 (Aug. 2011), 075463 (Cited 28 times). DOI: 10.1103/PhysRevB.84.075463.

2011

[12] Ahmet Artu Yıldırım and Cem Özdoğan. "Parallel WaveCluster: A linear scaling parallel clustering algorithm implementation with application to very large datasets". English. In: *Journal of Parallel and Distributed Computing* 71.7 (July 2011), 955–962 (Cited 6 times). DOI: 10.1016/j.jpdc.2011.03.007.

2011

[13] Jens Kunstmann, Cem Özdoğan, Alexander Quandt, and Holger Fehske. "Stability of edge states and edge magnetism in graphene nanoribbons". English. In: *Physical Review B* 83.4 (Jan. 2011), 045414 (Cited 191 times). DOI: 10.1103/PhysRevB.83.045414.

2011

[14] Ahmet Artu Yıldırım and Cem Özdoğan. "Parallel wavelet-based clustering algorithm on GPUs using CUDA". English. In: Procedia Computer Science 3 (2011). Ed. by A Karahoca and S Kanbul. 1st World Conference on Information Technology (WCIT), Bahcesehir Univ, Istanbul, Turkey, Oct 06-10, 2010, 396–400 (Cited 5 times). DOI: 10.1016/j.procs.2010.12.066.

2010

[15] Alexander Quandt and Cem Özdoğan. "Feynman, biominerals and graphene - Basic aspects of nanoscience". English. In: *Communications in Nonlinear Science and Numerical Simulation* 15.6 (June 2010), 1575–1582 (Cited 4 times). DOI: 10.1016/j.cnsns.2009.06.009.

2010

[16] Cem Özdoğan, Saikat Mukhopadhyay, W. Hayami, Ziya Burhanettin Güvenç, Ravindra Pandey, and Ihsan Boustani. "The Unusually Stable B-100 Fullerene, Structural Transitions in Boron Nanostructures, and a Comparative Study of alpha- and gamma-Boron and Sheets". English. In: *Journal of Physical Chemistry C* 114.10 (Mar. 2010), 4362–4375 (Cited 138 times). DOI: 10.1021/jp911641u.

2009
[17] Murat Atiş, Cem Özdoğan, and Ziya Burhanettin Güvenç. "Density Functional Study of Physical and Chemical Properties of Nano Size Boron Clusters: B-n (n=13-20)". English. In: *Chinese Journal of Chemical Physics* 22.4 (Aug. 2009), 380–388 (Cited 22 times). DOI: 10.1088/1674-0068/22/04/380-388.

2008
[18] Alexander Quandt, Cem Özdoğan, Jens Kunstmann, and Holger Fehske. "Boron doped graphene nanostructures". English. In: *Physica Status Solidi B* 245.10, SI (Oct. 2008), 2077–2081 (Cited 17 times). DOI: 10.1002/pssb.200879559.

2008
[19] Alexander Quandt, Cem Özdoğan, Jens Kunstmann, and Holger Fehske. "Functionalizing graphene by embedded boron clusters". English. In: *Nanotechnology* 19.33 (Aug. 2008), 335707 (Cited 20 times). DOI: 10.1088/0957-4484/19/33/335707.

2008
[20] Cem Özdoğan, Murat Atiş, and Ziya Burhanettin Güvenç. "Surface modification by 1 keV ion impact: molecular dynamics study of an Ar+-Ni(100) collision system". English. In: *Modelling and Simulation in Materials Science and Engineering* 16.3 (Apr. 2008), 035003 (Cited 0 time). DOI: 10.1088/0965-0393/16/3/035003.

2008
[21] Mustafa Böyükata, Cem Özdoğan, and Ziya Burhanettin Güvenç. "Effects of hydrogen hosting on cage structures of boron clusters: density functional study of B_mH_n ($m = 5 - 10$ and $n \leq m$) complexes". English. In: *Physica Scripta* 77.2 (Feb. 2008), 025602 (Cited 8 times). DOI: 10.1088/0031-8949/77/02/025602.

2008
[22] Mustafa Böyükata, Cem Özdoğan, and Ziya Burhanettin Güvenç. "Hydrogen hosting of nanoscale boron cluster". English. In: *Romanian Journal of Information Science and Technology* 11.1 (2008), 59–70 (Cited 3 times).

2007
[23] Gülay Dereli, Banu Süngü, and Cem Özdoğan. "Thermal stability of metallic single-walled carbon nanotubes: an O(N) tight-binding molecular dynamics simulation study". English. In: *Nanotechnology* 18.24 (June 2007), 245704 (Cited 8 times). DOI: 10.1088/0957-4484/18/24/245704.

2007
[24] Mustafa Böyükata, Cem Özdoğan, and Ziya Burhanettin Güvenç. "An investigation of hydrogen bonded neutral B4Hn (n=1-11) and anionic B4H11(-1) clusters: Density functional study". English. In: *Journal of Molecular Structure-THEOCHEM* 805.1-3 (Mar. 2007), 91–100 (Cited 23 times). DOI: 10.1016/j.theochem.2006.10.015.

2007
[25] Murat Atiş, Cem Özdoğan, and Ziya Burhanettin Güvenç. "Structure and energetic of B-n (n=2-12) clusters: Electronic structure calculations". English. In: *International Journal of Quantum Chemistry* 107.3 (Mar. 2007), 729–744 (Cited 46 times). DOI: 10.1002/qua.21171.

2005
[26] Murat Atiş, Cem Özdoğan, and Ziya Burhanettin Güvenç. "Parallelization of a molecular dynamics simulation of an ion-surface collision". English. In: *International Journal of Modern Physics C* 16.6 (June 2005), 969–990 (Cited 3 times). DOI: 10.1142/S0129183105007649.

2003
[27] Gülay Dereli and Cem Özdoğan. "O(N) algorithms in tight-binding molecular-dynamics simulations of the electronic structure of carbon nanotubes". English. In: *Physical Review B* 67.3 (Jan. 2003), 035415 (Cited 10 times). DOI: 10.1103/PhysRevB.67.035415.

2003
[28] Gülay Dereli and Cem Özdoğan. "Structural stability and energetics of single-walled carbon nanotubes under uniaxial strain". English. In: *Physical Review B* 67.3 (Jan. 2003), 035416 (Cited 66 times). DOI: 10.1103/PhysRevB.67.035416.

2002
[29] Cem Özdoğan, Gülay Dereli, and Tahir Çağın. "O(N) parallel tight binding molecular dynamics simulation of carbon nanotubes". English. In: *Computer Physics Communications* 148.2 (Oct. 2002), 188–205 (Cited 13 times). DOI: 10.1016/S0010-4655(02)00553-2.

1997
[30] Cem Özdoğan and Şakir Erkoç. "Molecular-dynamics simulation of the structural stability, energetics, and melting of Cu-n(n=13-135) clusters". English. In: *Zeitschrift fur Physik D-Atoms Molecules and Clusters* 41.3 (Aug. 1997), 205–209 (Cited 14 times).

- Web of Science Categories

Conference Publications

2018

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