CURRICULUM VITAE

Ch. E. Lekka

Department of Material Science & Engineering

Univeristy of Ioannina

Greece

Ioannina, November 2020

Curriculum Vitae

Christina E. Lekka

November 2020

Education

B.Sc. in Physics (1996), Physics Department, University of Ioannina, Ioannina, Greece

M.Sc. in Physics (1999), Physics Department, University of Ioannina, Ioannina, Greece, Thesis topic "Study of the vibrational and structural properties of the low index Cu_3Au surfaces with and without Cu or Au adatoms by Molecular Dynamics Simulations".

Ph.D. in Physics (2001), Physics Department, University of Ioannina, Ioannina, Greece, Thesis subject: "Computer simulation study of the properties of the ordered A_3B alloy surfaces (Cu_3Au, Ni_3Al)".

Professional positions

Postdoctoral Research assistant (2002) at the School of Computational Sciences, George Mason University, Fairfax VA, USA and the Center for Computational Materials Science, Naval Research Laboratory (NRL),Washington D.C., USA.

Teaching and research assistant (1-1-2003 until -31-8-2005): Materials Science and Engineering Department, University of Ioannina, Greece

Lecturer (31-8-2005 until 6-9-2009) at the Materials Science and Engineering Department, University of Ioannina, Greece

Assistant Professor (7-9-2009 until 7-7-2015) at the Materials Science and Engineering Department, University of Ioannina, Greece

Associate Professor (7-7-2015 until now) at the Materials Science and Engineering Department, University of Ioannina, Greece

Guest Professor in the Physics Dept., University of Vienna, Austria (May-June 2017): Teaching the course of "Computational Science of Nanoscaled Crystalline, Amorphous and Hybride Materials“ to undergraduate, MSc and Phd students also performing practical sessions in the Computer laboratory using the VASP (DFT) and the LAMMPS (MD) codes

Academic/Teaching experience:

Teaching experience:

Teaching courses at the Department of Materials Science and Engineering:

1. General Physics II (electricity-magnetism) (2003-until today,2nd semester, 4 ECTS units)
2. Atomic and electronic structure of solids (2003-until today,5τη semester, 4 ECTS units)
3. Applications of Information Technology (6th semester elective, 4 ECTS units)
4. Computational Methods in Materials Science (7th semester elective, 4 ECTS units)
5. Introduction to Advanced Computational Methods in Materials Science (9th semester elective, 4 ECTS units)

The courses' transparencies are available at http://cmsl.materials.uoi.gr/lekka/courses.html

Teaching the graduate courses at the Master Program " Advanced Materials":

6. "Atomic and Electronic Structure of Advanced Materials"
7. "Advanced computational material modeling"

Teaching the graduate courses at the Master Program " Materials Chemistry and Technology":

8. "Crystal structure – Mechanical and magnetic properties". Subject: Introduction to advanced computational methods in Chemistry and material science"

Author of University courses notes

1.1. Introduction to advanced computational methods in materials science (9ο semester, selective course, Number of Chapters 6 and number of pages 85)

1.2. Computational methods in material science (7ο semester, selective course, number of chapters 7 and number of pages 77), Co-author Prof. G.A.Evangelakis

Advisor in PhD Thesis:

1. M. Gialampouki: «Organic-inorganic hybridic nanomaterials with predetermined properties», (1-12-2010 – 28-2-2014) Current Postdoctoral fellow in Brown Univ. USA
2. G. Bokas, «Ab initio and semiempirical calculations on new nanostructured composite materials», (25.01.2011 – March 2014) Accepted for as Postdoctoral fellow in Wisconsin Univ. USA
3. J.J. Gutierrez Moreno, "Theory-guided bottom-up design of low-rigidity Ti-based alloys (ab initio and molecular dynamics calculations ", (10.03.2011 – 11.2014)
4. C. Cutrano, ' Computational design of functional Fe- and Cu- based coatings for environmentally sustainable applications', (Oct 2015 – 11.05.2020)
5. Y. Fortouna, " Antibacteria coatings of metallic surfaces: From ab-initio to large scale simulations", (5.2020 - until today

Member of the three member PhD committee of Dr L. Kutsokera, July 2010

Member of the seven member PhD committee of Dr D.Kilimi (2010), Dr G.Tziatzos (December 2010), Dr X. Zumbou (January 2012), in the Department of Materials Science and Engineering,

University of Ioannina and Dr E. Kalesaki, Department of Physics, Aristotle University of Thessaloniki (February 2012)

Advisor in Master Thesis:

1. M. Gialampouki, «Strustural and electronic properties of Ti nanoclusters on carbon nanotube or graphene by ab initio calculations», October 2010.
2. A. Balerba, «Structural properties and diffusion of graphene on Cu surfaces by molecular dynamics simulations », June 2013.
3. M. Bouri, « L-glutamin on Cu(111) surface by density functional theory», Jan 2015
4. M. Zegos «H_2O on Cu(111) surface by density functional theory,Feb 2016

Member of the three member Master committee of Mr. G. Almiras (2009), Ms A.Lagogianni (2009) and Mr G. Bokas (Nov 2010) at the Department of Physics, University of Ioannina

Advisor in the under graduated students final year thesis

1.1. Study of the structural and electronic properties of Fe – Flavonoids complexes (luteolin, 7,8 dihydroxyflavon, fisetin, quercetin) using DFTB calculations, Vasileiou H. April 2005

1.2. Study of the structural and electronic properties of Flavonoids without Fe chelating properties (Chrysin, 7-Hydroxyflavon, Flavon, 5-Hydroxyflavon) using DFTB, A.Kitsaki , April 2005

1.3. Structutal, electronic and vibrational properties of Cu nanowires with TB calculations and MD simulations, Z. Salta, June 2006

1.4. Study of the structural and electronic properties of Ti and Ti-O clusters on carbon nanotube by DFT calculations, M. Gialambouki, October 2008

1.5. Study of structural and electronic properties of Nb nanowires with TBMD calculations , M. Georgiadis, April 2009

1.6. Study of structural and electronic properties of Fe-O clustes on carbon nanotubes with DFT calculations S. Giorgi, November 2010

1.7. Study of structural and electronic properties of Metal nitridies using ab initio calculations, Th. Gouziotis, April 2011

1.8. Study of structural and electronic properties of Ti nanowires on carbon nanotudes by ab initio calculations, A. Balerba, October 2011

1.9. Study of structural and electronic properties of Cu nanowires on carbon nanotubes by ab initio calculations O. Gouma May 2012

1.10. Study of structural and electronic properties of Zn-flavonoids by DFT calculations, A. Kotsiopoulos Nov 2012

1.11. Growth of graphene flakes on Cu (001) surface by Molecular Dynamics Simulations, Kotanidis Alexios (AM. 951) Nov 2013

1.12. Structural and electronic properties of Ti-based alloys by ab initio calculations Papantoniou Alexios (AM. 687) July 2014

1.13. Growth of graphene flakes on Cu (111) surface by Molecular Dynamics Simulations,

Paraskeuas Aggelos (AM. 688) Nov 2019

1.14. Biocompatible Ti-based alloys by ab initio calculations, Aris Dimou (AM. 1219) Sept. 2019

1.15. Hybrids of Curcumin and Magnetic Fe-O nanoclusters by ab initio calculations, Eleni Kitsou (AM 1933) Nov 2019

Member in the thesis committee of several students with thesis advisors Assoc. Prof D. Papageorgiou, Assoc. Prof. E. Lidorikis and Assist. Prof. P. Patsalas.

Department administration committees

1.1. Economics (President since 2009)

1.2. Student's advisor committee (since 2010)

1.3. Graduate student's selecting examinations (since 2010)

1.4. Organizing the Department's Divisions (2009)

Research experience

Actual research interests

1. Study of the atomic and electronic structure of metals and theirs alloys, with or without defects, nanosized objects, biological molecules, metal/graphene or metal/CNT hybrids with the the Augmented Plane Wave (APW) theory, Density Functional theory (DFT) and the NRL-Tight Binding (NRL-TB) theory.
2. Study of structural, vibrational, mechanical and diffusion properties of metals and their alloys with classical semi-empirical molecular dynamics simulations (emphasis on metallic glasses, surface properties and nanosized objects)

Awards:

1. Poster award at the XIX National Solid State and Materials Science Conference, Thessaloniki, (21-24)-9-2003 for the presentation entitled "Electronic and optical properties of adsorbed biomolecules (adenine-cytosine)", by Ch.E. Lekka, G. Zonios, E. Kaxiras
2. Oral presentation award at the 14th ISMANAM2007, International Symposium on Metastable and Nano Materials, 26-30 August 2007, Chandris Hotel, Corfu, Chandris, Greece for the presentation entitled "Microscopic aspects of the deformation accommodation in the $Cu_{46}Zr_{54}$ Metallic Glass" by Ch.E. Lekka, L. Tayebi, A.R. Yavari, G.A. Evangelakis
3. Oral presentation award at the 6ο National Conference of "Free Radical and Antioxidant activity" Pramada (18-21)-9-2008, Greece for the presentation entitled: «Complexation of flavonoids with iron and Copper: Structure and Optical Signatures από τους Ch.E. Lekka, Jun Ren, Sheng Meng, Efthimios Kaxiras.
4. Poster award at the 27^{o} Panhellenic conference on solid state physics and materials science, Limassol, Cyprus, September 2011 στην εργασία «Structural and electronic properties of Ti-Nanowires/C-single wall nanotubes composites by Density functional theory calculations», M. Gialambouki, A. Balerba, Ch.E. Lekka
5. Best poster award, 19th International symposium on ISMANAM "Metastable, amorphous and nanostructured materials", 18-22 June 2012, Moscow, Russia, entitle «Structural, electronic and mechanical properties of Ti-Nbx (x<50) alloys», J.J. Gutiérrez Moreno, N. Panagiotopoulos, D.G. Papageorgiou, G.A.Evangelakis, Ch.E. Lekka, UoI and M. Bönisch, A. Helth, M. Calin, A. Gebert, M. Stoica, J. Eckert, IFW
6. Poster award at the 28ο Panhellenic conference on solid state physics and materials science, Patra, September 2012 στην εργασία «Al/Nb Microalloying effect and bonding particularities in the microstructure of Cu-Zr Metallic Glasses by ab-initio calculations», G. Bokas, G.A.Evangelakis, Ch.E. Lekka

Patent

A.T. Murdock, A.A. Koos, N. Grobert, C.E. Lekka, Process: Structural control of 2D nanomaterials produced by CVD on dedicated substrates, UK and US patent application filed March 2013, see Graphene Manufacture Technique: Isis Project No 8727 for further information.

Invited talks:

1. Conferencies :

1.1. Conference on Applied Surface Modeling: Experiment, Theory and Simulations, (21-23 August 2002), NASA, Cleveland, Ohio, USA: «Structural and electronic properties of the $Cu_3Au(111)$ surface», Ch.E. Lekka, N. Bernstein, M.J. Mehl and D.A. Papaconstantopoulos

1.2. Euronano BMG-Europe conference, Paris, 2-4 Dec, 2007 «Tensile deformation accommodation in microscopic metallic glasses via subnanocluster reconstructions», Ch.E. Lekka, A. Ibenskas, L. Tayebi, A.R. Yavari, G.A. Evangelakis

1.3. 16th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2009) Beijing, China, July 5 - 9, 2009, «On the origin of the short range order of the $Cu_{35}Zr_{65}$ and $Cu_{65}Zr_{35}$ metallic glass, Ch.E. Lekka, G. Almyras, N. Mattern, G.A. Evangelakis

1.4. WPI-Europe Workshop on Metallic Glasses and Related Materials, 25-28 August 2009, Grenoble, France, «Bonding characteristics and strengthening of CuZr fundamental clusters upon small Al additions», Ch. E. Lekka, G. A. Evangelakis

1.5. ISMANAM 2011, 26June-1July, Gijon, Spain, «Clustering and mechanical properties in Cu/Zr-based glassy models by Molecular Dynamics and ab-initio computations», Ch.E. Lekka, G.B. Bokas, G.A. Almyras, D.G. Papageorgiou, G.A. Evangelakis

1.6. ISMANAM 2013, 1-5 July, Torino, Italy, «Ti-Nb phase transitions from electronic structure calculations» Ch.E. Lekka , J.J. Gutierrez-Moreno , G.A.Evangelakis , M. Boenisch , M. Calin , J. Eckert

1.7. Euromat 2013, 8-13 September, Sevilla, Spain, "Al/Nb Microalloying effect and bonding particularities in the microstructure of Cu-Zr Metallic Glasses by ab-initio calculations", G. B. Bokas, G.A. Evangelakis, Ch.E. Lekka

1.8. 30th Panhellenic Conference on Solid-State Physics and Materials Science, September 21-24, 2014, Heraklion, Biocompatible Titanium-based alloys for orthopaedics, Ch.E. Lekka (invited)

1.9. 2018 Materials Research Society MRS Spring Meeting & Exhibit , Phoenix, Arizona, 2-6 April 2018,"On the Design of Fe-X (X=Cu, Co, Mn) Nanoclusters and Coatings with Improve Magnetic Moment by Density Functional Theory Calculations", C. Cutrano and Ch. E. Lekka

1.10. 9th International Conference on Materials Scie & Cond Matter Physics (MSCMP2018), Chsinau, Moldavia, 25-28 September 2018, "Density functional theory on nanostructures with potential catalytic applications", Ch. E. Lekka (Plenary speaker)

1.11. 2018 Sustainable Industrial Processing Summit & Exhibition (SIPS2018), Rio de Janeiro, Brazil, 4-7 November 2018, "On The Computational Design Of Ti- and Fe-Based Advanced Materials For Biomedical Applications", Ch. E. Lekka

1.12. ISFOE19, 12th International Symposium on Flexible Organic Electronics, 1-4 July 2019, Thessaloniki, Greece, "Density functional theory on Nanostructures with potential catalytic applications" and "Women in Nano", Martha Gialampouki, Ch.E. Lekka

2. University or Institude:

2.1. Harvard University, Boston 25 August 2002, USA: «Structural, vibrational and electronic properties of Cu_3Au surfaces by Tight Binding Molecular Dynamics Simulations», Ch.E. Lekka

2.2. IFW Dresden, Germany 6 Nov. 2007, «Atomistic mechanisms of the deformation accommodation in microscopic CuZr Metallic Glasses», Ch.E. Lekka

2.3. Naval Research Laboratory, Washington DC, Feb 22, 2008, USA: «Atomistic Mechanisms Of The Deformation Accommodation In Microscopic CuZr Metallic Glass», Ch.E. Lekka

2.4. National Hellenic Research Foundation, 10 June 2010, Athens, «Short-Range order, bonding characteristics and mechanical properties of Cu-Zr Metallic Glass Models; effects of Al or Nb minor substitutions», Ch.E. Lekka

2.5. Department of Materials, University of Oxford, Begbroke Science Forum, November 2011, «Ti_N decoration of Single Wall Carbon Nanotubes and Graphene by Density Functional Theory Computations», M. A. Gialampouki and Ch.E. Lekka

2.6. IFW Dresden, Germany 3 March 2014, "Metallic glasses and alloys from electronic structure calculations" Ch. E. Lekka

2.7. Chemisch, Physikalishe, Gessellschaft, Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien, 13 June 2017, Metal - graphene / carbon nanotube hybrids by density functional theory, Ch.E. Lekka

2.8. Materials Physics, University of Leoben, Austria 16 June 2017, Clustering and mechanical properties in Cu/Zr-based glassy models by Molecular Dynamics and ab-initio computations,

2.9. Guest Professor in the Physics Dept., University of Vienna, Austria (May-June 2017): Teaching the course of "Computational Science of Nanoscaled Crystalline, Amorphous and Hybride Materials" to undergraduate, MSc and Phd students also performing practical sessions in the Computer laboratory using the VASP (DFT) and the LAMMPS (MD) codes

Research projects :

1. H2020-MSCA-ITN-2019, project No 861046, 2020 - 2023, BIOfilm-REsistant Materials for hard tissue Implant Applications (BIOREMIA)
2. H2020-MSCA-ITN-2014, project No 642642, 2015-2018, Smart ELECTrodeposited Alloys for environmentally sustainable applications: from advanced protective coatings to micro/nano-robotic platforms (SELECTA)
3. e-COST, European Cooperation in the field of Scientific and Technical Research (044/13) TARGET Network 1301 (2013-2015): Next generation of Young Scientist: towards a contemporary spirit of R&I (Sci-Generation), Member of the Management committee
4. FP7-PEOPLE-2010-ITN, (No 264635), 2011-2014, Academic-Industrial Initial Training Network on Innovative Biocompatible Titanium-based Structures for Orthopaedics (BioTiNet) (Responsible of the UoI group, budget 217787.50 euro)
5. FP7-SiS-2008-1 (No 230253), 2009-2011, Science in Society, Improving the gender diversity management in materials research institutions (Diversity), (Responsible of the UoI group, budget 8300 euro)
6. UoI Research Committee Program, 2007-2009 (No. 80018) «Nanowires and nanoclusters of catalytic metallic oxides from oxygen plasma: From ab-initio calculations to experimental synthesis», (budget 6000 euro)
7. Participation in European research projects: (ITN VITRITECH 2014, RNT Marie Curie 2001, RNT Marie Curie 2003, European Space Agency 2007) as well as National projects (PENED96, Pythagoras 2003)

Organizing Conferences

1. Gateway to Academics: Materials modelling for target applications, SELECTA workshop, 3-7 September 2017, Ioannina
2. XXXII Panhellenic Conference on Solid State Physics and Materials Science, 18-21 September 2016, Ioannina
3. Workshop 'Science Communication & Presentation' 17-18 /9/ 2012 και BioTiNet MidTerm meeting, 19-21 /9/2012, (Organizer) Chandris Dasia Hotel, Corfu, Greece
4. European Workshop: "Women in European Materials Science Research Institutions" (Organizer), DIVANI, Corfu 19-20 May 2011
5. 28ο Panhellenic conference on solid state physics and materials science, 26-29 September 2010, Ioannina (Financial Secretary)
6. 14th ISMANAM2007, International Symposium on Metastable and Nano Materials, 26-30 August 2007, Chandris Hotel, Corfu, Chandris, Greece (Member of the local organizing committee) and Satellite meeting of WomenInNano (Organizer), 28 August 2007– Corfu , Chandris, Greece
7. Workshop on "Recent developments on Bulk Metallic Glasses", 25 June 2004 – Corfu, Hotel Corfu Palace, Greece (Member of the local organizing committee)

Main research collaborators :

1. Prof. M. Calin, Dr A. Gebert, Dr. N. Mattern, Prof. J. Eckert, IFW, Dresden, Germany
2. Prof. D.A. Papaconstantopoulos George Mason University, Virginia, USA (Naval Research Laboratory, Washington D.C)
3. Prof. E. Kaxiras, Harvard Univeristy, Boston, USA
4. Prof. G. A. Evangelakis, University of Ioannina
5. Prof. N. Grobert, Oxford University , UK

Visits in foreign Institutes :

1. Center for Computational Materials Science, Naval Research Laboratory, Washington D.C., May 8th-21st 2000. Purpose of visit: Application of the NRL-tight-binding method to bcc metals and Cu-Au alloys. Collaboration with Prof. D.A. Papaconstantopoulos and Prof. M.Mehl.

2. CINECA High performance Systems Division, Casalecchio di Reno, Bologna, Italy., Dates: September 25th-October 20th 2000 and April 30th - May 12th 2001. Award of a MINOS project: Multidisciplinary Intensive Computing for Research Activities of European Scientists. Purpose of visit: Application of the NRL-tight-binding molecular dynamics simulations for Nb bcc metal. Performance of TBMD code on the Cray T3E platform and validate the method by calculating some bulk properties for Nb.
   The report of the project will be publiced in CINECA's Icarus magazine “Daedalus”:
   1. "Vibrational properties of the Nb bcc by Tight Binding Molecular Dynamics Simulations", Ch.E.Lekka, Daedalus 2001, 1.
   2. "Vibrational and structural properties of the Nb (001) bcc surface by Tight Binding Molecular Dynamics Simulations", Ch.E.Lekka, Daedalus 5 2001, 5.
   3. School of Computational Sciences at George Mason University, Fairfax, Virginia. Collaboration with Prof. D.A. Papaconstantopoulos and Dr. M.Mehl
   1. December 26th- February 9th 2004. Purpose of visit: Study of the universality of the NRL-tight-binding parameters of bcc metals and their alloys.
   2. July 24th -31st August 2005. Purpose of the visit: Apply the NRL-TBMD on bcc metals with defects and their nanoclusters.
   4. Department of Physics, Harvard University, Boston, USA, 31 January – 13 Febrary 2006. Purpose of the visit: Study the interaction of biological molecules with metallic ions with density functional theory calculations. Collaboration with Prof. E. Kaxiras
   5. IFW Dresden, Germany 4-8 Nov. 2007. Research collaboration with Prof. J. Eckert and N. Mattern on the study of CuZr metallic glass (theoretical versus experimental data of the radial distribution function).
   6. 10-23 Feb. 2007, USA, George Mason University, Fairfax,VA και Harvard Univ. Boston. Collaboration with Prof. D. A. Papaconstantopoulos and E. Kaxiras, respectively
   7. November 2011 and June 2011, Department of Materials, Oxford University, Research collaboration with Prof. N. Grobert on the graphen growth on Cu substrates.
   8. IFW Dresden, Germany July 2012. Research collaboration with Prof. J.Eckert and Prof. M. Calin on the study of Ti-based alloys within the BioTiNet project.

List of Publications :

1. Self-diffusion processes of Cu adatom on Cu(110) surface by Molecular Dynamics Simulations, G.A. Evangelakis, D.G. Papageorgiou, G.D. Kallinteris, Ch.E. Lekka, N.I. Papanikolaou, Vacuum, **50**, 165 (1998) – (Impact factor (IF=0.909)),
2. Diffusion processes of Au and Cu adatoms on the $C_{u3}Au$(001) surface, Ch. Lekka, G.A. Evangelakis, Surf. Sci. **473** (2001) 39. (IF=1.78),
3. Transferability of Slater-Koster parameters, Ch.E .Lekka, N.I. Papanicolaou, G.A. Evangelakis, D.A. Papaconstantopoulos, J. Phys. and Chem. Solids. **62** (2001) 753. (IF=1.41)
4. Molecular dynamics study of the ordered Cu_3Au. I Vibrational and structural properties of the low-indexed Cu3Au surfaces by Molecular Dynamics Simulations, Ch.E.Lekka, N.I. Papanicolaou, G.A.Evangelakis, Surf. Sci. **479** (2001) 287. (IF=1.78)
5. Molecular dynamics study of the ordered Cu_3Au. II Vibrational properties of the Cu and Au adatoms on the ordered low-index Cu_3Au surfaces by Molecular Dynamics Simulations, Ch.E.Lekka, N.I. Papanicolaou, G.A.Evangelakis, Surf. Sci. **488** (2001) 269. (IF=1.78)
6. Vacancy diffusion driven Cu_3Au and Ni_3Al (001) surface re-arrangement, Ch.E. Lekka, G.A. Evangelakis, Appl. Surf. Sci. **9509** (2002) 1. (IF=1.263)
7. Molecular Dynamics study of the transport and structural properties of the Cu_3Au(110) and Ni_3Al(110) surface, Ch.E.Lekka, D.G.Papageorgiou, G.A.Evangelakis Surf. Sci. **518** (2002) 111. (IF=1.78)
8. Molecular Dynamics study of Cu and Au 2D adlayers on the Cu_3Au(110) surface, D.G.Papageorgiou, Ch.E.Lekka, G.A.Evangelakis, Appl. Surf. Sci. **219** (2003) 64. (IF=1.263)
9. Transport processes and structural properties of the Cu_3Au and Ni_3Al(111) surface by Molecular Dynamics, Ch.E. Lekka, D.G. Papageorgiou and G.A. Evangelakis, Surf. Sci. 541 (2003) 182. (IF=1.78)
10. Electronic structure of the Cu_3Au(111) surface, Ch.E. Lekka, N. Bernstein, M.J. Mehl and D.A. Papaconstantopoulos, Appl. Surf. Sci. 219 (2003) 158. (IF=1.263)
11. Tight binding molecular dynamics simulations of Nb surfaces and surface defects, Ch.E. Lekka, M.J. Mehl, N. Bernstein, D.A. Papaconstantopoulos, Phys. Rev. B68 (2003) 35422. (IF=3.185)
12. Electronic, Structural and Thermodynamic properties of icosahedral free and supported Al clusters on Al surfaces from Tight Binding and classical Molecular Dynamics simulations, P. Mitev, D.G. Papageorgiou, Ch.E. Lekka and G.A. Evangelakis, Surf.Sci. 566-568 (2004) 937. (IF=1.78)
13. Mechanical properties of nano-grained Zr_2Ni systems bu molecular dynamics simulations, G.A. Evangelakis, D.G.Papageorgiou, Ch.E.Lekka, I.E. Lagaris, J.Alloys and Comp. 434-435 (2007) 546. (IF=2.289)
14. Structural, Thermodynamic and Mechanical properties of Zr based binary nanowires (ZrCu and Zr_2Ni) by Molecular Dynamics, A. Ibenskas, Ch.E. Lekka and G.A. Evangelakis, Physica B37 (2007) 189 (IF=0.796)
15. Structure and dynamics of the Ni3Al low index surfaces with and without Ni/Al adatoms from Molecular Dynamics Simulations, Ch.E. Lekka, G.A. Evangelakis, Materials Chemistry and

Physics 103, 2-3 (2007) 500. (IF=1.136)Structural and electronic properties of V, Nb and Ta nano-clusters by Tight Binding Molecular Dynamics Simulations, Ch.E. Lekka, D.A. Papaconstantopoulos, Surf.Sci. **601** (2007) 3937 (IF=1.78) Oxidation of the Nb(110) surface by ab-initio calculations" by D.A.Kilimis and Ch.E.Lekka, Materials Science and Engineering B144 (2007) 27 (IF=1.33)

18. Tensile deformation accommodation in microscopic metallic glasses via subnanocluster reconstructions, Ch.E. Lekka, A. Ibenskas, A.R. Yavari, G.A. Evangelakis, Appl.Phys.Lett. 91 (2007) 214103 (IF=4.127)
19. Molecular Dynamic Simulations of Zr_2Ni(100) surface in presence of Ni or Zr adatoms, Ch.E. Lekka and G.A. Evangelakis, Surf. Sci 602, (2008) 590-596 (IF=1.78)
20. Complexation of Flavonoids with Iron, J.Ren, S. Meng, Ch.E. Lekka, E.Kaxiras, J. Phys. Chem. B, 112 (6), 1845 -1850, 2008 (IF=4.033)
21. Structural and vibrational properties of deposited Cu or Zr surface adlayers on Cu46Zr54 bulk metallic glass, D.G. Papageorgiou, A. Ibenskas, Ch.E. Lekka and G.A. Evangelakis, Rev.Adv.Mater.Sci.18(2008) 98 (IF=1.12)
22. Conducting transition metal nitride thin films with tailored cell sizes: the case of δ-TixTa1-xN, L.E. Koutsokeras, G. Abadias, Ch.E. Lekka, G.M. Matenoglou, D.F. Anagnostopoulos, G.A. Evangelakis and P. Patsalas APL **93** (2008) 011904 (IF=4.127)
23. Poisson ratio under compressive and tensile strain; effect on the mechanical response of the Cu46Zr54 metallic glass, L. Tayebi Ch. E. Lekka and G. A. Evangelakis, Physica Status Solidi (A) Applications and Materials, 205 (2008) 2603 (IF = 1.214)
24. L.Tayebi, Ch.E. Lekka, G.A. Evangelakis,Journal of alloys and compounds, 483 (2009) 570–572 (IF=2.289)
25. Structural characteristics of CuxZr1-x metallic glasses by Molecular Dynamics Simulations, A.E. Lagogianni, G. Almyras, Ch.E. Lekka, D.G. Papageorgiou, and G.A. Evangelakis, Journal of Alloys and Compounds 483 (2009) 658–661 (IF=2.289)
26. Static and Dynamic Tight-Binding Simulations of the Binary NbMo and CuZr alloys, Ch. E. Lekka, D. A. Papaconstantopoulos, M.J. Mehl, Daniel Finkenstadt, G. Evangelakis, Journal of Alloys and Compounds 483 (2009) 627–631 (IF=2.289)
27. Optical properties, structural parameters, and bonding of highly textured rocksalt tantalum nitride films, G. M. Matenoglou L. E. Koutsokeras, Ch. E. Lekka,G. Abadias, S. Camelio, G. A. Evangelakis, C. Kosmidis,3 and P. Patsalas, JAP 104 (2008) 124907 (IF=2.168)
28. Deformation induced directional amorphization in Zr2Ni systems: a remedy for the mechanical failure of nano-crystalline alloys Ch.E. Lekka, D.G. Papageorgiou, G.A. Evangelakis J. Nanosci. Nanotechnol. 9 (2009) 1-7 (IF=1.987)
29. Structural, electronic and optical properties of representative Cu-flavonoid complexes, Ch. E. Lekka, Jun Ren, Sheng Meng, Efthimios Kaxiras, J. Phys. Chem. B 2009, 113, 6478–6483 (IF=4.033)

30. Properties of BCC Metals by Tight Binding Total Energy Simulations, Ch. E. Lekka, N. Bernstein, D. A. Papaconstantopoulos, M. J. Mehl, Materials Science and Engineering B 163 (2009) 8–16 (IF=1.33)
31. Structure and electronic properties of conducting, ternary TixTa1-xN films, G.M. Matenoglou, Ch.E. Lekka, L.E. Koutsokeras, G. Karras, C. Kosmidis, G.A. Evangelakis and P. Patsalas, Journal of applied physics 105, 2009, 103714 - 103718 (IF=2.168)
32. Structure, stability and bonding of ternary transition metal nitrides, G. M. Matenoglou; Loukas E Koutsokeras, Ch. E. Lekka, G. Abadias, C. Kosmidis, G. A Evangelakis, P.A. Patsalas, Surface Coating and Technology 204 (2009) 911-914 (IF = 1.867)
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    47.1. «Ti-Nb phase transitions from electronic structure calculations» Ch.E. Lekka , J.J. Gutierrez-Moreno , G.A.Evangelakis , M. Boenisch , M. Calin , J. Eckert (προσκεκλημένη ομιλία)
    47.2. Al-Nb bonding particularities upon microalloying Cu-Zr based Metallic Glasses by ab-initio calculations, G.B. Bokas, G.A. Evangelakis, Ch.E. Lekka (αφίσα)
    47.3. On the role of Icosahedral-like clusters in the solidification and the mechanical response of Cu-Zr metallic glasses by Density Functional Theory, G.B. Bokas, G.A. Almyras, A.E. Lagogianni, Ch.E. Lekka, D.G. Papageorgiou, G.A. Evangelakis (αφίσα)
    47.4. Structural and electronic properties of β-Ti-40Nb-xIn (x < 25 w%), J.J. Gutierrez-Moreno, G.B. Bokas, Ch.E. Lekka, A. Helth, M. Bonisch, A. Gebert, M. Calin, J. Eckert(αφίσα)
    47.5. Structural, electronic and mechanical properties of β-Ti-Nb-Sn alloy: Experiment versus ab-initio calculations, J.J. Gutierrez-Moreno, G.A. Evangelakis, Ch.E. Lekka, Yaofeng Guo, A. R. Yavari (αφίσα)
48. Euro LightMat 2013, 03-05 September, Bremen, Germany, "Biocompatible Ti-xNb (14 < x< 40) alloys: Structural, electronic and mechanical properties", J.J. Gutiérrez Moreno, G.A. Evangelakis, D.G. Papageorgiou, Ch.E. Lekka, M. Boenisch, M. Calin, A. Gebert, J. Eckert (ομιλία)
49. Euromat 2013, 8-13 September, Sevilla, Spain,

49.1. "Al/Nb Microalloying effect and bonding particularities in the microstructure of Cu-Zr Metallic Glasses by ab-initio calculations", G. B. Bokas, G.A. Evangelakis, Ch.E. Lekka (προσκεκλημένη ομιλία)

49.2. Biocompatible Ti-Nb and Ti-Nb-Hf thin films by magnetron sputtering and ab-initio calculations, N.T. Panagiotopoulos, J.J. Gutierrez-Moreno, P. Patsalas, Ch.E. Lekka, G.A. Evangelakis (αφίσα)

50. NT13, 14th International Conference on the Science and Application of Nanotubes, 14-26 June 2013

50.1. Ti Decoration of Single Wall Carbon Nanotubes and Graphene by Density Functional Theory Computations, M.A. Gialampouki and Ch.E. Lekka (αφίσα)

50.2. Early Stages of Ti-O Clusters' Growth on CNTs by Ab-initio Calculations, M.A. Gialampouki and Ch.E. Lekka (αφίσα)

51. 14^{th} International Conference on Intergranular and Interphase Boundaries in Materials "ibb2013", June 23-29, 2013 Halkidiki, Greece

51.1. Structural properties and diffusion processes of graphene flakes growing on Cu(110), A.V. Balermpa, D.G. Papageorgiou, Ch.E. Lekka, Adrian T. Murdock, Antal Koos, Nicole Grobert (αφίσα)

51.2. Phase transition processes in Ti, Zr, Hf and their Ti-based biocompatible alloys A.V. Balermpa, A.E. Lagogianni, J.J. Gutierrez Moreno, Ch.E. Lekka, D.G. Papageorgiou, G.A. Evangelakis (αφίσα)

52. 8th Biotinet workshop, 4-8 Nov. 2014, Dresden , Ti-based alloys for orthopaedics, J.J.Gutierrez Moreno, Ch.E. Lekka (oral)

53. 'Fundamentals of electrodeposition of metallic alloys: state-of- the-art at European and International levels', Solaris Resort, Vrnjacka Banja, Serbia, November 2015, Fe-Cu coating on Cu surfaces by Density Functional Theory, C. Cutrano, Ch.E. Lekka (oral)

54. 'Training on research methodologies, characterization techniques and reporting scientific results', IFW Dresden, Germany, March 2016, oral pres: 'Fe-Cu coating on Cu(001) by Density Functional Theory' C. Cutrano, Ch.E. Lekka (oral)

55. 'Micro and nano-electrodeposition for MEMS/NEMS and micro/nano-robotic platforms. Overview of lithography methods. Impact to society', HP, Wiener Neustadt, Austria, August 2016, oral pres: 'Cu-Fe nanoclusters and Fe/Cu(111) by density functional theory' C. Cutrano, Ch.E. Lekka (oral)

56. Selecta Mid-Term review meeting and Workshop, Göteborg Sweden, December 2016, oral pres: 'Design of functional dense and nanoporous Fe-, Al- and Cu-based coatings by molecular dynamics simulations and DFT calculations' C. Cutrano, Ch.E. Lekka (oral)

57. 10th International Summer Schools on N&N, OE & NM (ISSON16), 2-9 July 2016, Thessaloniki, Greece, 'Fe-Cu coating on Cu(001) by Density Functional Theory' C. Cutrano, Ch.E. Lekka

58. ISMANAM 3-8 July 2016, Nara, Japan,

58.1. Structural and electronic properties of biocompatible Ti-based alloys, Ch. E. Lekka,

J.J.Gutierrez-Moreno, G.A. Evangelakis (oral)

58.2. Structural, magnetic and electronic properties of CuFe nanoclusters by density functional theory calculations, Ch. E. Lekka, C. S. Cutrano (poster)

59. Gateway to Academics: Materials modelling for target applications, University of Ioannina, 3-7 September 2017, Fe-X (X=Mn, Co, Cu) nanoclusters by density functional theory calculations, C. Cutrano, Ch.E. Lekka (poster)
60. CECAM summer school: Teaching the Theory in Density Functional Theory, Lausanne, 12-16 June 2017 Fe-X (X=Mn, Co, Cu) nanoclusters by density functional theory calculations, C. Cutrano, Ch.E. Lekka (poster)
61. EUROMAT 2017: "Nanoscale Materials Characterization and Modelling by Advanced Microscopy Methods", Thessaloniki Greece, September 2017
    61.1. Electronic origin and structural instabilities of Ti-based alloys suitable for orthopaedic implants, Ch.E. Lekka, J.J. Gutiérrez-Moreno, M. Calin (oral)
    61.2. Fe-X (X=Mn, Co, Cu) nanoclusters by density functional theory calculations, C. Cutrano, Ch.E. Lekka (Poster Presentation)
    61.3. Nano-Hybrids of Curcumin And Fe-based clusters by density functional theory, K. N. Botsiou, D. G. Karantzinis, Ch. E. Lekka (poster)
62. Gateway to Industry: Introducing materials to market. Practical aspects, Cambridge, 7-12 January 2018, Fe-X (X=Mn, Co, Cu) nanoclusters by density functional theory calculations, C. Cutrano, Ch.E. Lekka (poster)
63. 'Advanced magnetic materials and devices for biomedical applications', Torino, 21-25/05/2018, Fe-X (X=Mn, Co, Cu) nanoclusters by density functional theory calculations, C. Cutrano, Ch.E. Lekka (Oral Presentation)
64. SPSSM 2018: 7Th International symposium on Structure-Property relationship in solid state materials, Pescara, 8-12/06/2018, Structural and magnetic properties od Fe-X (X=Co,Cu) nanoclusters by density functional theory calculations, C.Cutrano, C. Lekka (Poster Presentation)
65. ISMANAM 2018, Roma, 2-6/07/2018, Structural and magnetic properties od Fe-X (X=Co,Cu) nanoclusters by density functional theory calculations, C.Cutrano, C. Lekka (Poster Presentation)
66. 'Overview of the SELECTA achievement. Final Reporting', Barcelona, 26-29/08/2018, Structural and magnetic properties od Fe-X (X=Co,Cu) nanoclusters by density functional theory calculations, C.Cutrano, C. Lekka Oral presentation
67. EUFEPS Annual meeting 2018, 24-26 May 2018, Athens, Nano-Hybrids of Curcumin And Fe-based nano-clusters by density functional theory, Ch. E. Lekka
68. 2018 Materials Research Society MRS Spring Meeting & Exhibit , Phoenix, Arizona, 2-6 April 2018,"On the Design of Fe-X (X=Cu, Co, Mn) Nanoclusters and Coatings with Improve Magnetic Moment by Density Functional Theory Calculations", C. Cutrano and Ch. E. Lekka (invited)
69. 9th International Conference on Materials Scie & Cond Matter Physics (MSCMP2018), Chsinau, Moldavia, 25-28 September 2018, "Density functional theory on nanostructures with potential catalytic applications", Ch. E. Lekka (Plenary speaker)
70. 2018 Sustainable Industrial Processing Summit & Exhibition (SIPS2018), Rio de Janeiro, Brazil, 4-7 November 2018, "On The Computational Design Of Ti- and Fe-Based Advanced Materials For

Biomedical Applications", Ch. E. Lekka (invited)

71. ISFOE19, 12th International Symposium on Flexible Organic Electronics, 1-4 July 2019, Thessaloniki, Greece, "Density functional theory on Nanostructures with potential catalytic applications" and "Women in Nano", Martha Gialampouki, Ch.E. Lekka (invited)
72. EETSY Workshop on Computational Materials Science, 14-15 Dec 2019, Thessaloniki, On The Computational Design Of Ti- and Fe-Based Advanced Materials For Biomedical Applications, Christina E. Lekka, J.J. Gutierrez Moreno, C. Cutrano, K. Ioannou, D. Papageorgiou, G. Evangelakis.

Participation in National conferences:

1. XII Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ηράκλειο, Κρήτη (15-18)-9-1996 «Δυναμικές ιδιότητες του προσροφημένου ατόμου Au στις χαμηλών δεικτών επιφάνειες του Cu με προσομοιώσεις Μοριακής Δυναμικής», Γ.Χ.Καλλιντέρης, Χ.Ε.Λέκκα, Ν.Ι.Παπανικολάου, Γ.Α.Ευαγγελάκης (αφίσα)
2. ΙΓ Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Θεσσαλονίκη (15-18)-9-1997 «Διαδικασίες διάχυσης των προσροφημένων ατόμων Cu στην επιφάνεια Cu(110) με προσομοιώσεις Μοριακής Δυναμικής», Γ.Α.Ευαγγελάκης, Δ.Γ. Παπαγεωργίου, Γ.Χ. Καλλιντέρης, Χ.Ε. Λέκκα, Ν.Ι. Παπανικολάου. (αφίσα)
3. XIV Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ιωάννινα, (15-18)-9-1998:
   3.1. «Ταλαντωτικές ιδιότητες των χαμηλών δεικτών των επιφανειών του Cu_3Au με ή χωρίς προσροφημένα άτομα Cu/Au με προσομοίωση Μοριακής Δυναμικής», Χ.Ε.Λέκκα, Γ.Α.Ευαγγελάκης, Ν.Ι.Παπανικολάου (αφίσα)
   3.2. «Δυνατότητα μεταφοράς των παραμέτρων της θεωρίας ισχυρού δεσμού σε ένα μεταβατικό στοιχείο (Nb)», Χ.Ε. Λέκκα, Ν.Ι. Παπανικολάου, Γ.Α. Ευαγγελάκης, Δ.Α. Παπακωνσταντόπουλος (αφίσα)
4. XVI Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ναύπλιο, (17-20)-9-2000, «Διαδικασίες διάχυσης των προσροφημένων ατόμων Au και Cu στην επιφάνεια $Cu_3Au(001)$», Χ.Ε. Λέκκα, Γ.Α. Ευαγγελάκης (αφίσα)
5. XVII Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Θράκη, (6-9)-9-2001:
   5.1. «Διάχυση οπών και ατομική τάξη στην επιφάνεια $Cu_3Au(001)$», Χ.Ε.Λέκκα, Γ.Α.Ευαγγελάκης (παρουσίαση ομιλίας).
   5.2. «Μελέτη της συμπεριφοράς σημειακών ατελειών (προσροφημένα άτομα ή οπές) στην επιφάνεια (001) των κραμάτων τύπου A_3B», Χ.Ε. Λέκκα, Γ.Α. Ευαγγελάκης. (αφίσα)
6. XIX Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Θεσ/ικη,(21-24) – 9 -2003:
   6.1. «Προσομοιώσεις θεωρίας ισχυρής δέσμευσης επιφανειών Nb με ή χωρίς επιφανειακές ατέλειες», Χ.Ε.Λέκκα, M.J.Mehl, N.Bernstein, D.A.Papaconstantopoulos (παρουσίαση ομιλίας)

6.2. «Ηλεκτρονιακές, δομικές και θερμοδυναμικές ιδιότητες ελευθέρων και προσροφημένων εικοσαεδρικών νανοσυσσωματωμάτων Al σε επιφάνειες Al με θεωρία ισχυρής δέσμευσης και προσομοιώσεις μοριακής δυναμικής», P.Mitev, Δ.Γ.Παπαγεωργίου, Χ.Ε.Λέκκα, Γ.Α. Ευαγγελάκης. (αφίσα)

6.3. «Οπτικές και ηλεκτρονιακές ιδιότητες προσροφημένων βιολογικών μορίων (αδενίνη, κυτοσίνη) σε φύλλο γραφίτη» Χ.Ε. Λέκκα, Γ. Ζώνιος, Ε. Καξίρας. (αφίσα)

7. XX Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ιωάννινα, (26-29)-9-2004

7.1. Structural and electronic properties of flavonoids, H. Basileiou, A. Kitsaki, Ch. E. Lekka, D. Galaris, E. Kaxiras (αφίσα)

7.2. Structural and electronic properties of C nanotubes, P. Theodorakis, Ch.E. Lekka, E. Kaxiras (αφίσα)

7.3. Molecular dynamics simulation of $Ni_xAl_{(1-x)}$ nanocluster deposited on Al(111) surface, P. Euthimiopoulos, D.G. Papageorgiou, Ch. E. Lekka, E. Kaxiras (αφίσα)

7.4. Structural and electronic properties of Ni, Al, NiAl, Ni_3Al and $NiAl_3$ nanoclusters, D. Kilimis, Ch.E. Lekka, D. G. Papageoriou, E. Kaxiras (αφίσα)

8. XXII Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Πάτρα (24-27)-9-2006

8.1. Molecular Dynamic Simulations of $Zr_2Ni(100)$ surface in presence of Ni or Zr adatoms, Ch.E. Lekka and G.A. Evangelakis (αφίσα)

8.2. Structural, Thermodynamic and Mechanical properties of Zr based binary nanowires (ZrCu and Zr_2Ni) by Molecular Dynamics, A. Ibenskas, Ch.E. Lekka and G.A. Evangelakis (αφίσα)

8.3. Structural and electronic properties of V, Nb and Ta nano-clusters by Tight Binding Molecular Dynamics Simulations, Ch.E. Lekka, D.A. Papaconstantopoulos (ομιλία)

9. 6ο Πανελλήνιο Συνέδριο Ελευθέρων Ριζών και Οξειδωτικού Στρες, Πράμαντα (18-21)-9-2008, «Complexation of flavonoids with iron and Copper: Structure and Optical Signatures από τους Ch.E. Lekka, Jun Ren, Sheng Meng, Efthimios Kaxiras (ομιλία)

10. XXIV Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Κρήτη 21-24 Σεπτ. 2008

10.1. Atomistic Mechanisms Of The Deformation Accommodation In Microscopic CuZr Metallic Glass, Ch.E.Lekka, A.R. Yavari, G.A. Evangelakis (ομιλία)

10.2. Structural And Electronic Properties Of Ti And TiO2 On C Nanotubes By Ab-Inio Calculations, M.Gialampouki and Ch.E.Lekka (αφίσα)

10.3. Structural and Electronic Properties Of Nb Nanowires By Tight Binding Molecular Dynamics Calculations, M. Iakovidis, Ch.E.Lekka (αφίσα)

10.4. Complexation of Flavonoids with Iron and Copper: Structure and Optical Signatures, Ch. E. Lekka, Jun Ren, Sheng Meng, Efthimios Kaxiras (αφίσα)

11. 6^{ov} Πανελλήνιο Πολυμερών, Ιωάννινα 28 Σεπτ.-1Οκτ. 2008

11.1. Structural And Electronic Properties Of Ti And TiO2 On C Nanotubes By Ab-Inio Calculations, M.Gialampouki and Ch.E.Lekka (αφίσα)

11.2. Structural and Electronic Properties Of Nb Nanowires By Tight Binding Molecular Dynamics Calculations, M. Iakovidis, Ch.E.Lekka (αφίσα)

12. XXIV Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Θεσσαλονίκη 21-24 Σεπτ. 2009
    12.1. Ultra Fine Structure of the Sort Range Order of the Cu65Zr35 and Cu35Zr65 Metallic Glasses, Ch. E. Lekka, G. Almyras, G.A .Evangelakis (ομιλία)
    12.2. CuZr nanoclusters by ab-inition calculations, G. Bokas, Ch.E. Lekka, G. A. Evangelakis (αφίσα)
    12.3. Structural and electronic properties of octahedral Titanium Oxide on Graphene by ab-initio calculations, M.Gialampouki and Ch.E.Lekka (αφίσα)
    12.4. Structural and Electronic Properties of Metal Nitrides, Th. A. Goutziotis, L. E. Koutsokeras, P. Patsalas and Ch. E. Lekka (αφίσα)
13. Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης και επιστήμης των υλικών, 26-29 Σεπτεμβρίου, Ιωάννινα 2010
    13.1. Structural and Electronic Properties of Ti adatom and Clusters on C Nanotubes and Graphene by ab-initio Calculations, M. Gialampouki and Ch.E. Lekka (αφίσα)
    13.2. Structural and electronic properties of CuxZr12-xY (Y=Be, Mg, Al, Si, P, Nb, Ag) clusters by ab-inio calculations, G. Bokas, G.A. Evangelakis, Ch.E.Lekka (αφίσα)
    13.3. Ti Nanowires on and inside Carbon Nanotubes by ab-initio Calculations: A Structural and Electronic Properties study, A. Mbalerba and Ch. E. Lekka (αφίσα)
    13.4. Structural and Electronic Properties of Fe Nanowires on and inside Carbon Nanotubes by Ab-Initio Calculations, S. Giorgi and Ch.E. Lekka (αφίσα)
    13.5. Ab-Initio Calculations of Cu Nanowires on and inside Carbon Nanotubes: A study of the Structural and Electronic Properties, O. Gouma and Ch. E. Lekka (αφίσα)
    13.6. Fine structure of short range order in CuxZr100-x metallic glasses by Molecular Dynamics Simulations, G.A. Almyras, Ch.E. Lekka, D.G. Papageorgiou, N. Mattern and G.A. Evangelakis (αφίσα)
    13.7. Complexation of Flavonoids with Zn: Structural and Electronic Properties, A.P. Kotsiopoulos and Ch.E. Lekka (αφίσα)
14. Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης και επιστήμης των υλικών, ΚΥΠΡΟΣ
    14.1. Ti_N decoration of Single Wall Carbon Nanotubes and Graphene by Density Functional Theory Computations, M. Gialampouki and Ch.E. Lekka (ομιλία)
    14.2. Ultra Thin Metallic Nanowires Templated on/in Single-Wall Carbon Nanotubes by Density Functional Theory Calculations, M.A. Gialabouki, A. Balerba, O. Gouma, Ch.E. Lekka (αφίσα)
15. Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης και επιστήμης των υλικών, ΠΑΤΡΑ 2012
    15.1. Stability and Bonding Characteristics of Fe and Ti Oxides on Single Wall Carbon Nanotube by Density Functional Theory Computations, M.A. Gialampouki and Ch.E. Lekka (αφίσα)
    15.2. Al/Nb Microalloying effect and bonding particularities in the microstructure of Cu-Zr Metallic Glasses by ab-initio calculations, G.B. Bokas, G.A. Evangelakis and Ch.E. Lekka (αφίσα)
16. XXIX Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης και επιστήμης των υλικών, 22-25 Σεπτεμβρίου Αθήνα 2013
    16.1. On the role of Icosahedral-like clusters in the solidification and mechanical response of Cu-Zr metallic glasses by Density Functional Theory, G. B. Bokas, G. A. Almyras, A. E. Lagogianni, Ch. E. Lekka, D. G. Papageorgiou, G. A. Evangelakis (ομιλία)
    16.2. Early Stages of Ti-O clusters growth on SWCNTs by Density Functional Theory Calculations, M. A. Gialampouki, Ch. E. Lekka (ομιλία)
    16.3. CO_2 adsorption on TiN/Graphene systems (N=1, 3, 13) by ab-initio Calculations, M.

A.Gialampouki, Ch. E. Lekka (αφίσα)

16.4. Biocompatible Ti-xNb (14<x<40) alloys: Structural, electronic and mechanical properties, J. J. Gutierrez Moreno, D. G. Papageorgiou, G. A. Evangelakis, Ch. E. Lekka, M. Boenisch, A.Helth, A. Gebert, M. Calin, J. Eckert (αφίσα)

17. XXIX Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης και επιστήμης των υλικών, 22-25 Σεπτεμβρίου Αθήνα 2013

17.1. On the role of Icosahedral-like clusters in the solidification and mechanical response of Cu-Zr metallic glasses by Density Functional Theory, G. B. Bokas, G. A. Almyras, A. E. Lagogianni, Ch. E. Lekka, D. G. Papageorgiou, G. A. Evangelakis (ομιλία)

17.2. Early Stages of Ti-O clusters growth on SWCNTs by Density Functional Theory Calculations, M. A. Gialampouki, Ch. E. Lekka (ομιλία)

17.3. CO_2 adsorption on TiN/Graphene systems (N=1, 3, 13) by ab-initio Calculations, M. A.Gialampouki, Ch. E. Lekka (αφίσα)

17.4. Biocompatible Ti-xNb (14<x<40) alloys: Structural, electronic and mechanical properties, J. J. Gutierrez Moreno, D. G. Papageorgiou, G. A. Evangelakis, Ch. E. Lekka, M. Boenisch, A.Helth, A. Gebert, M. Calin, J. Eckert (αφίσα)

18. 30th Panhellenic Conference on Solid-State Physics and Materials Science, September 21-24, 2014, Heraklion, Biocompatible Titanium-based alloys for orthopaedics, Ch.E. Lekka (invited)

19. XXXI Panhellenic Conference on Solid State Physics and Materials Science, Thessaloniki, 20-23, September 2015

19.1. L-glutamine on Cu(111) surface by Density Functional Theory Calculations, M. G. Bouri and Ch. E. Lekka (poster presentation)

19.2. Density Functional Theory Calculations of H2O Adsorption on Cu(111), Manos Zegkos and Ch.E. Lekka (poster presentation)

20. XXXII Panhellenic Conference on Solid State Physics and Materials Science, 18-21 September 2016, Ioannina, Structural, magnetic and electronic properties of CuFe nanoclusters by density functional theory calculations, C. Cutrano, Ch.E. Lekka (poster presentation)