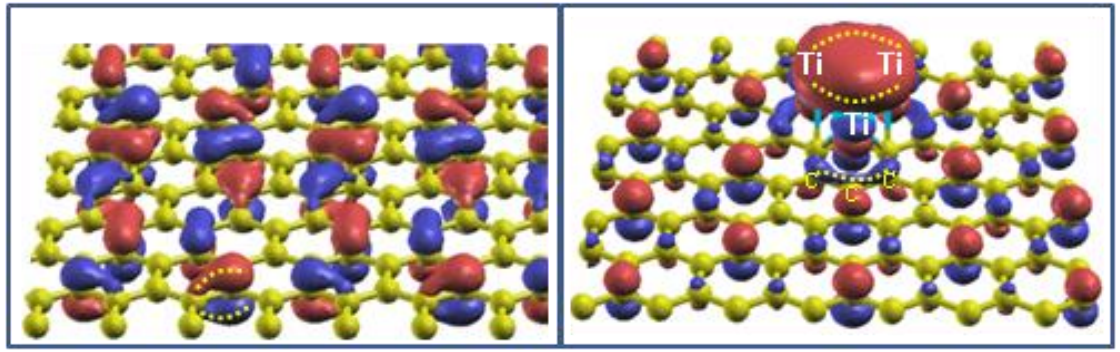
UOI
Πανεπιστήμιο Ιωαννίνων
Τμήμα Μηχανικών Επιστήμης Υλικών
Εργαστήριο Υπολογιστικής Επιστήμης Υλικών
INSTITUTE OF MATERIALS SCIENCE AND COMPUTING

Ατομική και ηλεκτρονιακή δομή των υλικών



Χριστίνα Λέκκα
Αναπλ. Καθηγήτρια

Εργαστήριο Υπολογιστικής Επιστήμης Υλικών

http://cmsl.materials.uoi.gr

Προσωπικό

- ✓ 3 μέλη ΔΕΠ + 2 ΕΔΙΠ
- ✓ 2 Post-Doc + 10 PhD
- ✓ 3 MSc + 6 BSs / έτος

Στόχοι

- ✓ μελέτη δομής και ιδιοτήτων υλικών
- ✓ σχεδιασμός υλικών & διατάξεων
- ✓ ανάπτυξη λογισμικών προσομοίωσης

Συνολική χρηματοδότηση:

- ✓ αρχική επένδυση: ~0.1 M€
- ✓ τακτικός προϋπ.: ~0.1 M€
- ✓ ανταγωνιστική: ~3.5 M€

Δραστηριότητα

Μελέτη υλικών:

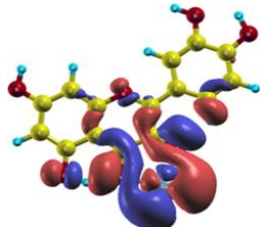
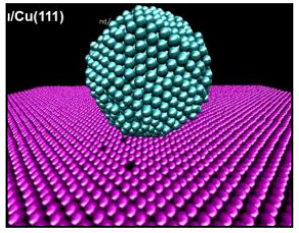
- ηλεκτρονιακή δομή
- μοριακή δυναμική
- μεταφορά φορτίου ή θερμότητας
- αλληλεπιδράσεις φωτός

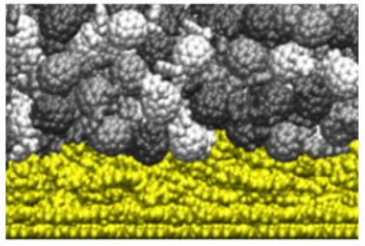
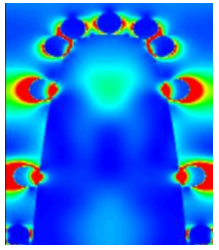
Εφαρμογές:

- νανοϋλικά, βιοϋλικά
- οργανικά ηλεκτρονικά
- ανιχνευτές & αισθητήρες
- φωτοβολταϊκά



μόρια *νανοσωματίδια* *νανοδομές* *νανοδιατάξεις*

10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} μέτρα

Υποδομές:

- 600 υπολογιστικοί πυρήνες
- 2 φοιτητικά εργαστήρια 36 θέσεων
- 3 ερευνητικά εργαστήρια 12 θέσεων

Ch. E. Lekka, UoI

Computational methods

Quantum mechanics

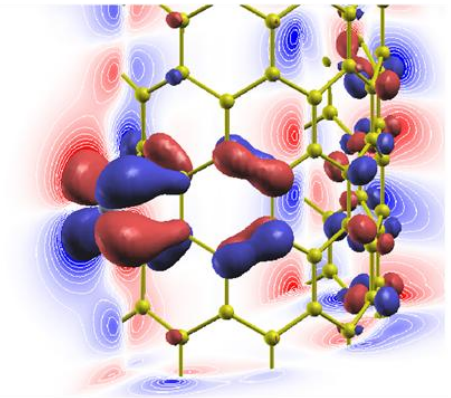
Classical mechanics

Ab-initio

Density functional theory

< 350 atoms

(VASP, WIEN2k, SIESTA)



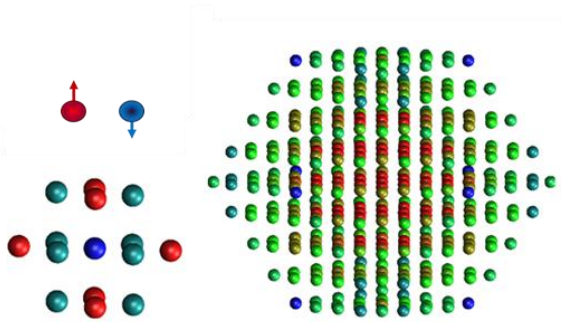
Ti on (8,0)

Semi ab-initio

Tight Binding

< 3000 atoms

(US Naval Research Lab TB)



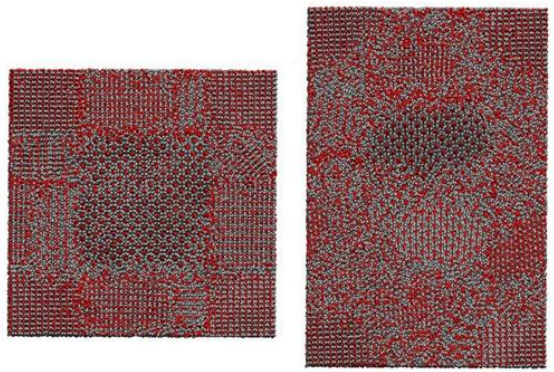
Nb's charge transfer

Classical

Molecular Dynamics

1000 – 10^9 atoms

(Lammps, Home made code)



Nanostructured ZrNi

Å → nm

Length scale

Βιολογικά μόρια

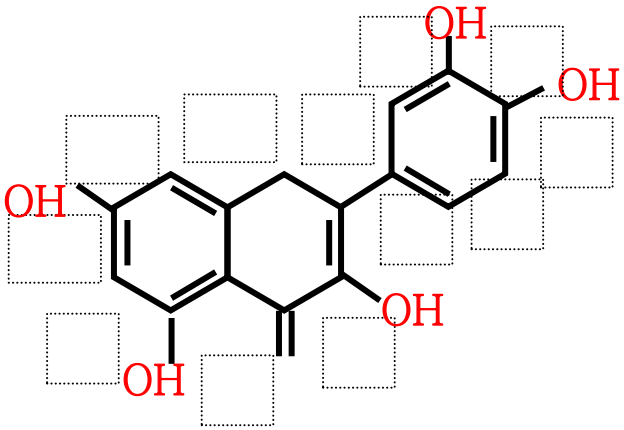
Φλαβονοειδή

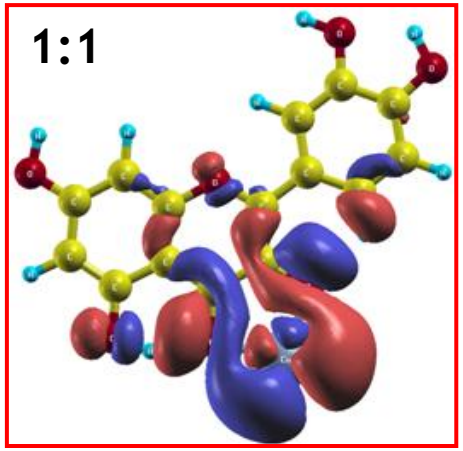


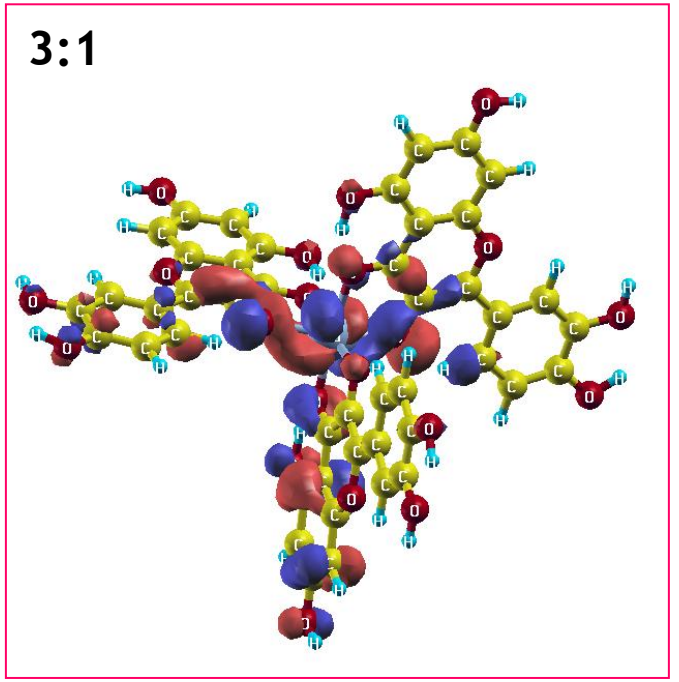


Prof. E. Kaxiras
Harvard Univ

Αύξηση της αντιοξειδωτικής δράσης λόγω της δέσμευσης μεταλλικών ιόντων



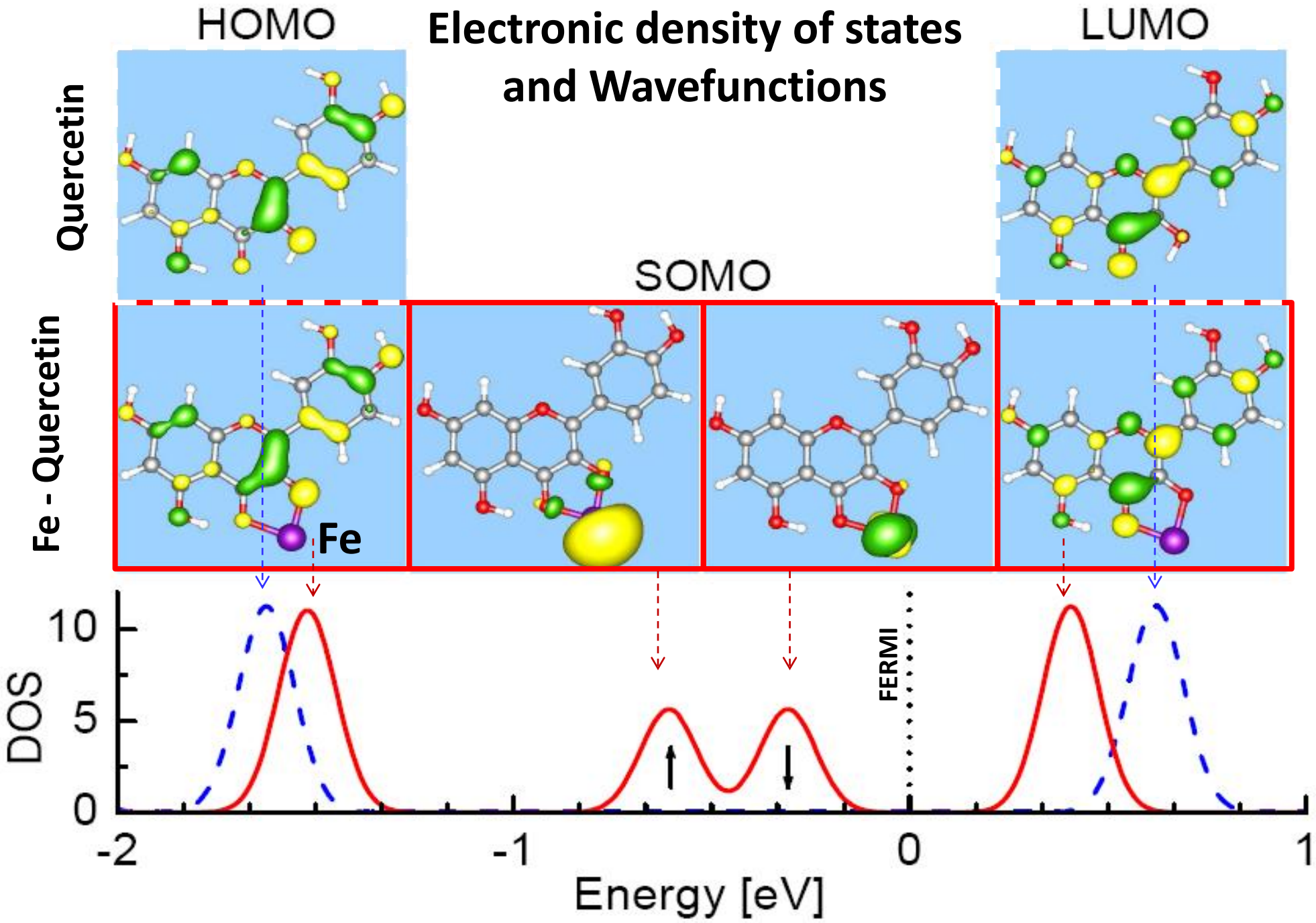




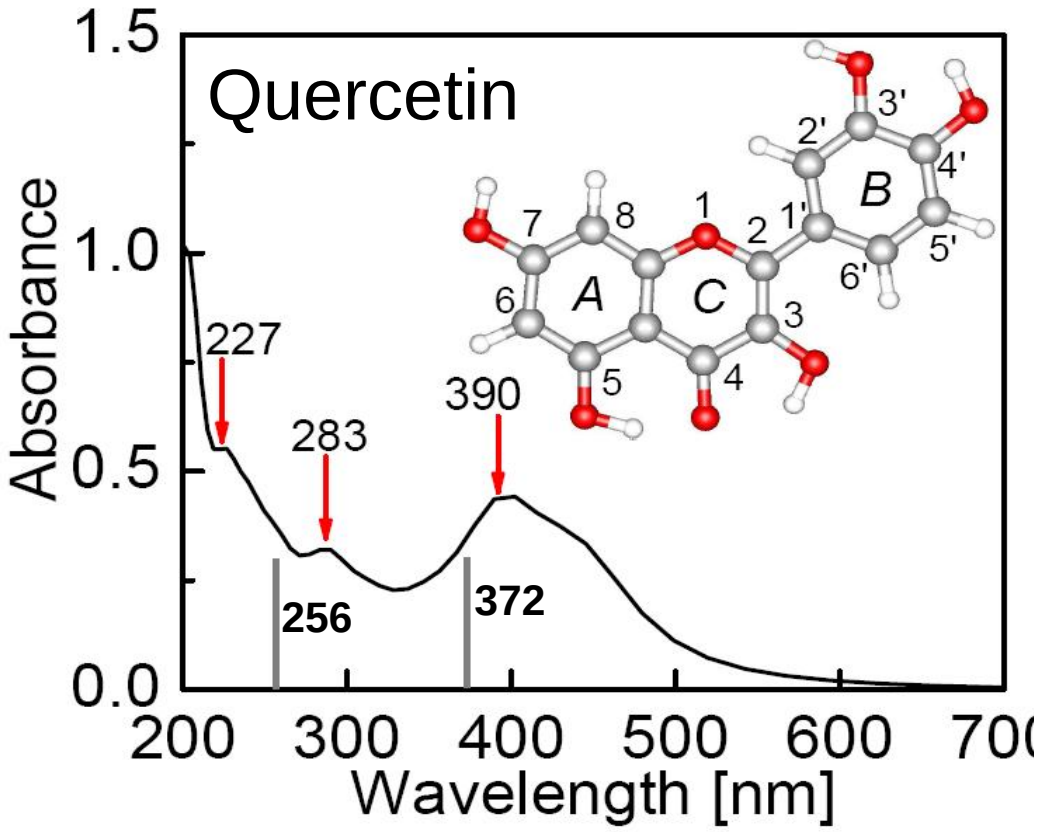
Prof. Galaris
Univ Ioannina

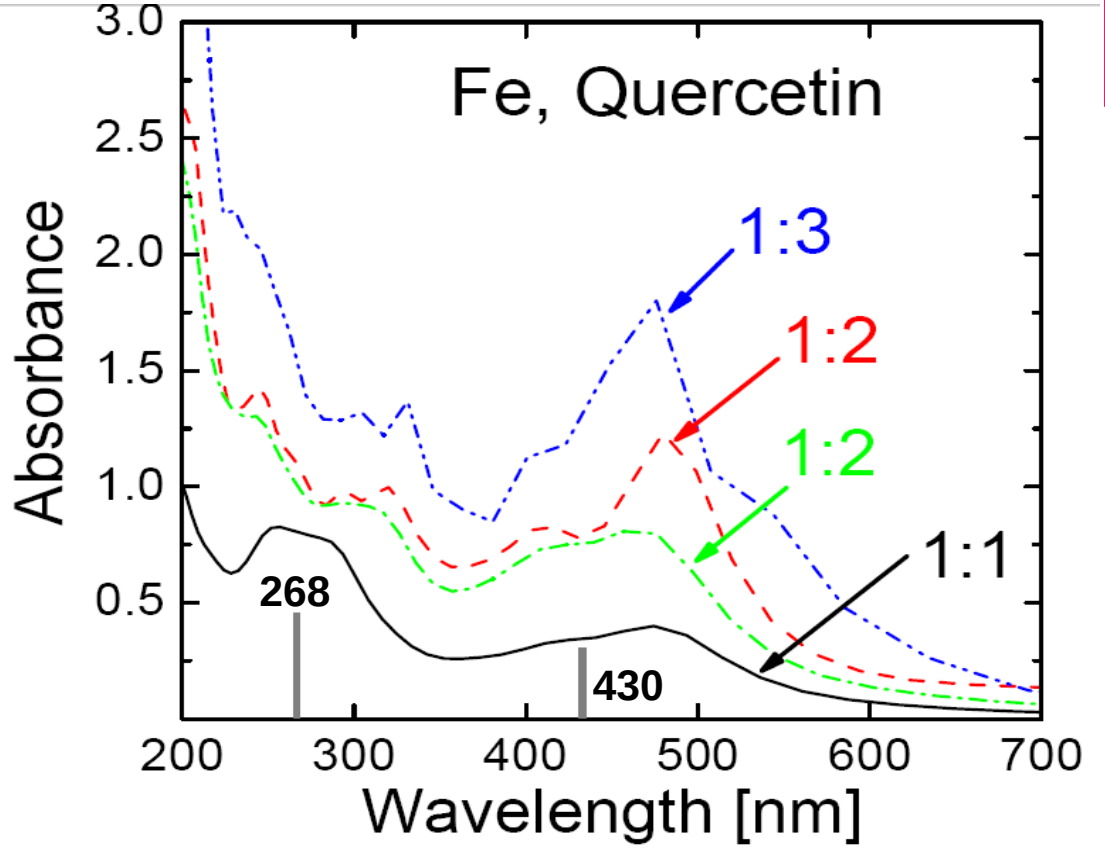
Protection against nuclear DNA damage offered by flavonoids in cells exposed to hydrogen peroxide: the role of iron chelation.
Melidou, M.; Riganakos, K.; Galaris, D. Free Radic. Biol. Med. 2005, 39, 125

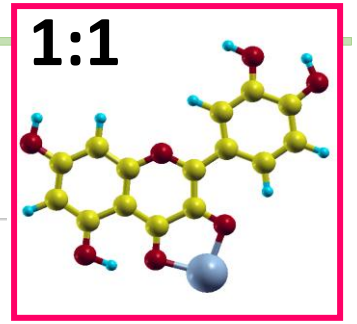
Electronic density of states and Wavefunctions

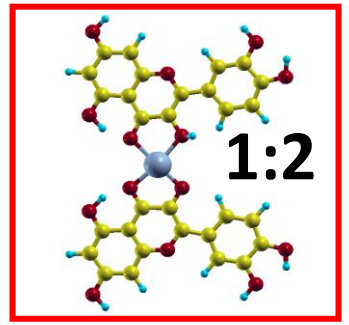


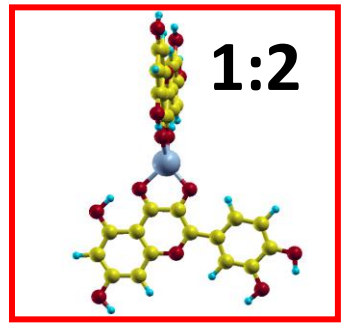
Optical adsorption (UV-vis)

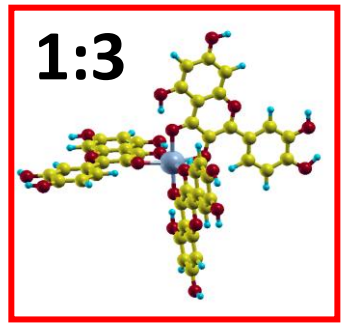








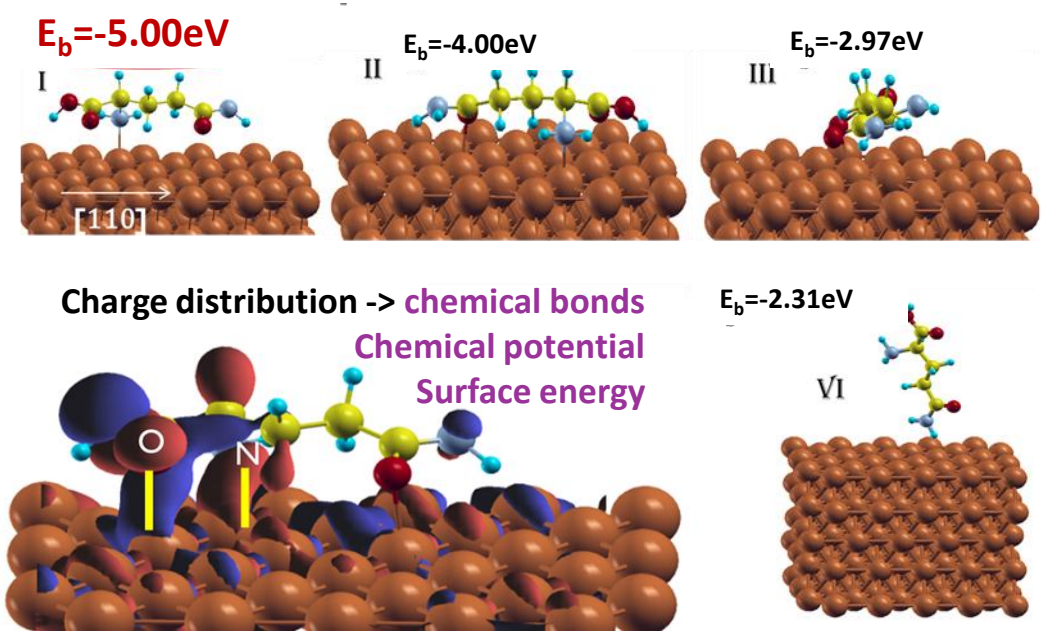




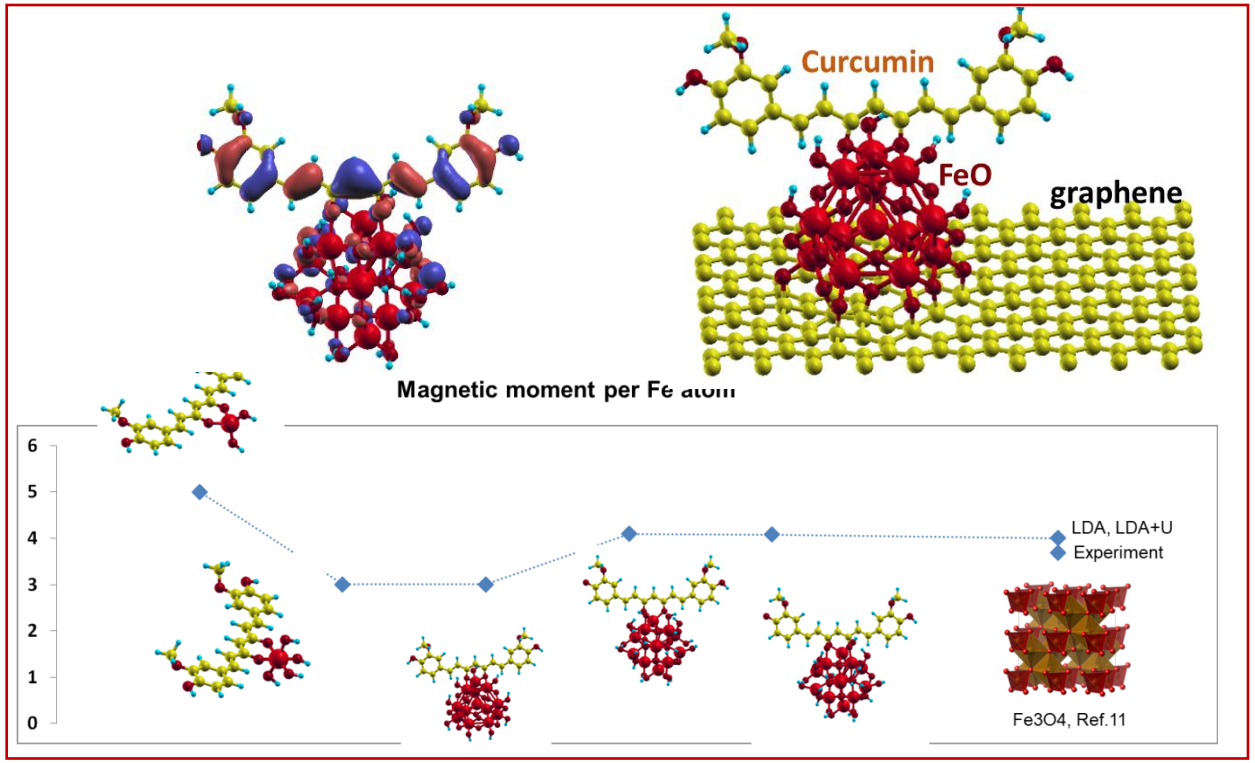
1. Complexation of **Flavonoids with Iron**, J.Ren, S. Meng, Ch.E. Lekka, **E.Kaxiras,** J. Phys. Chem. B, 112 (6), 1845 -1850, 2008
2. Structural, electronic and optical properties of representative **Cu-flavonoid** complexes, Ch. E. Lekka, Jun Ren, Sheng Meng, **Efthimios Kaxiras**, J. Phys. Chem. B 2009, 113, 6478–6483
3. Understanding **Zn(II) Chelation with Quercetin** and Luteolin: a Combined NMR and Theoretical Study, A Primikyri, E Sicilia, Ch Lekka, **A Tzakos**, N Russo, **I.P. Gerothanassis**, J. Phys. Chem. B119 (2015), 83-95

Molecule's adsorption sites

L-glutamine on Cu(111)



Curcumin on FeO nanocluster



Master Thesis of Dr M. Bouri, 2015

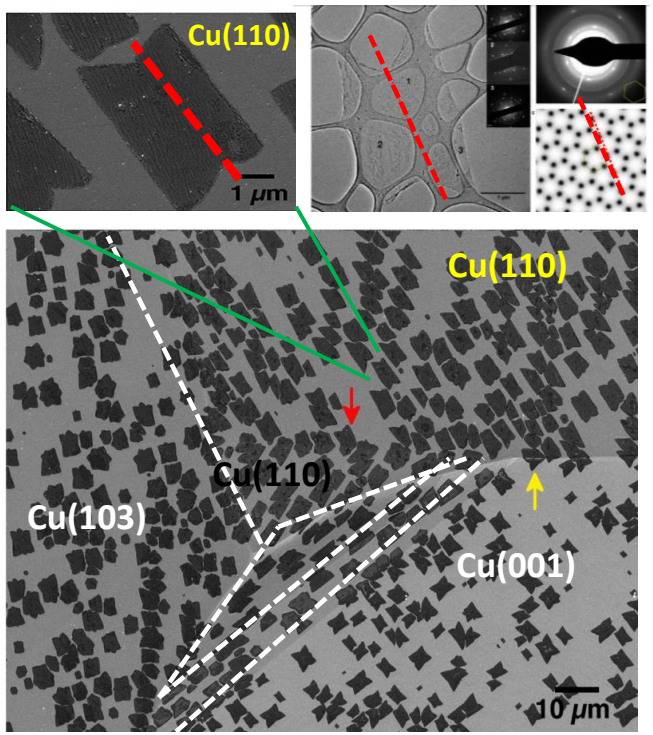
PhD at University of Bern, Switzerland

Undergraduate Thesis of E. Kistou, 2019

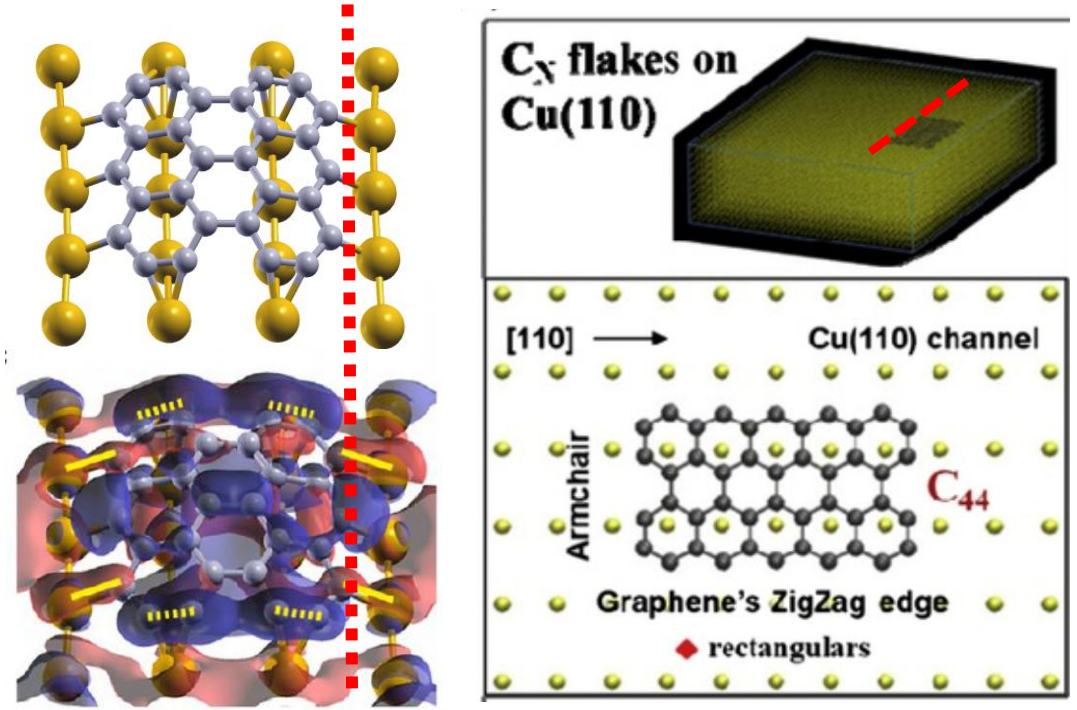
Controlling the Orientation, Edge Geometry, and Thickness of Chemical Vapor Deposition Graphene

Prof. N.Grobert,
Materials Depart.
Univ. Oxford

Graphene flakes on Cu



Experimental work,Uni. Oxford
***ACS Nano* 7 (2), 2013, 1351-1359**



Ab-initio theory and Classical Molecular Dynamics Simulations
(Book Chapter) Frontiers of Nanoscience, **2020**, 17, pp. 141-159

Patent: Intellectual property due diligence form, Isis project 8727: Structural control of 2D nanomaterials produced by CVD on dedicated substrates, University of Oxford. Inventors: Mr Adrian Murdock (25%), Dr Antal Koos (25%) and Prof Nicole Grobert (25%) University of Oxford and Contributor: Assist.Prof. Christina Lekka (25%), University of Ioannina

Metallic Nanostructures on CNTs and Graphene

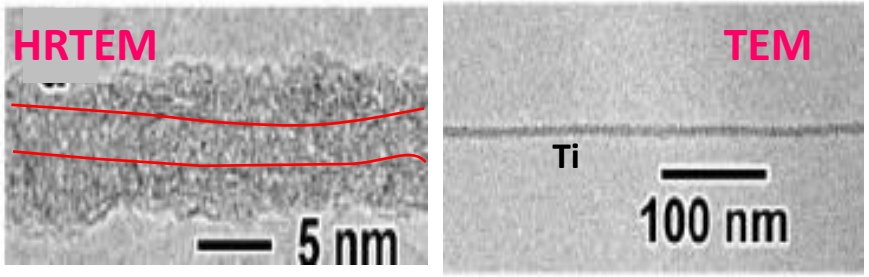
Dr. Martha Galampouki
Project Officer of H2020

These hybrid materials may exhibit different properties (structural, electronic etc.) depending on the type of metallic adsorbent.

The metallic coating on CNTs

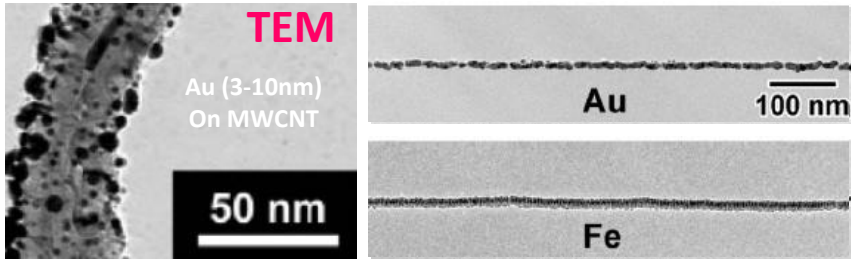
continuous coating

(e.g. Ti, Nb, Ta)



clusters

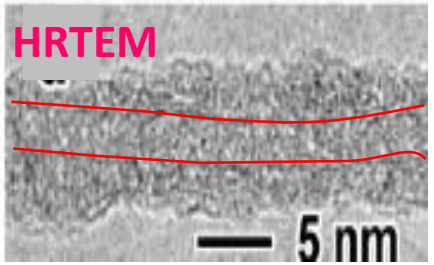
(e.g. Au, Fe, Cu)



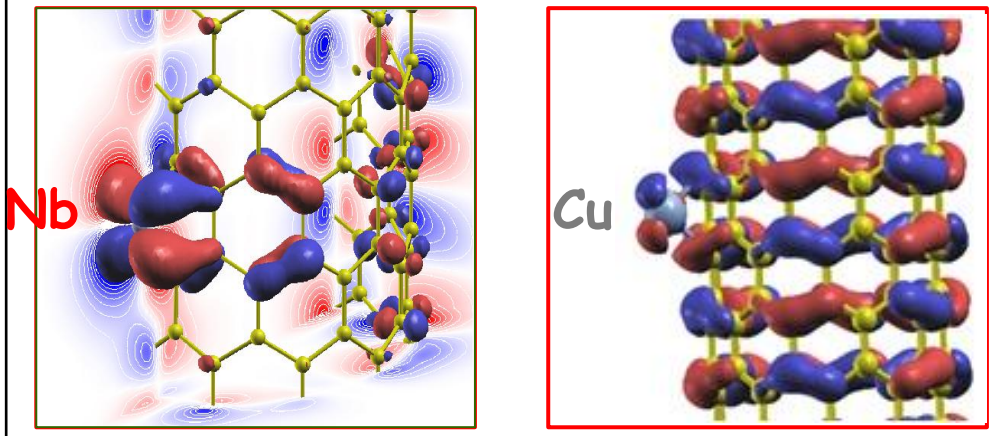
[1] Georgakilas V., D. Gournis et al. J. Mater. Chem. 2007, 17, 2679
[2] Zhang Y. et al Appl. Phys. Let. 2000, 77, 3015
[3] Durgun, E.et al T. Phys. Rev. B 2008, 77, 08540
[4] Yildirim, T. et al. Phys. Rev. Lett. 2005, 94, 175501

Metallic Nanostructures on CNTs and Graphene

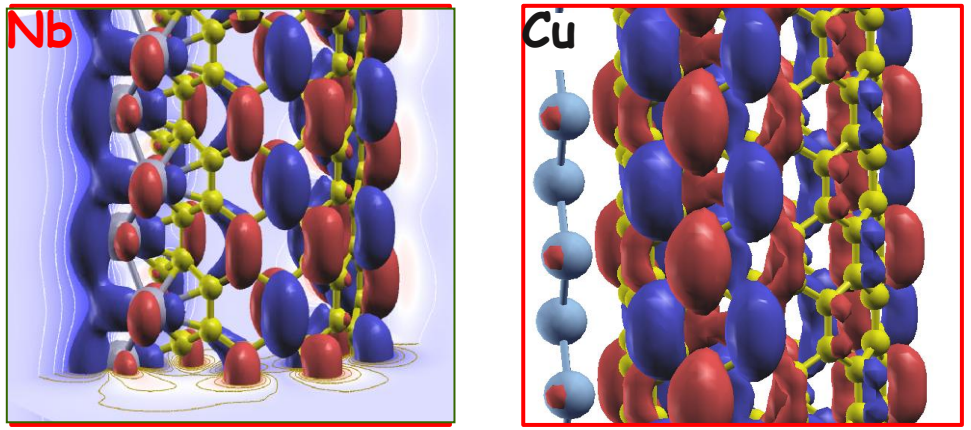
Nb/Ti



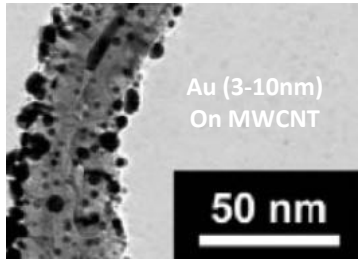
Atoms on CNT



Atomic nanowire on CNT

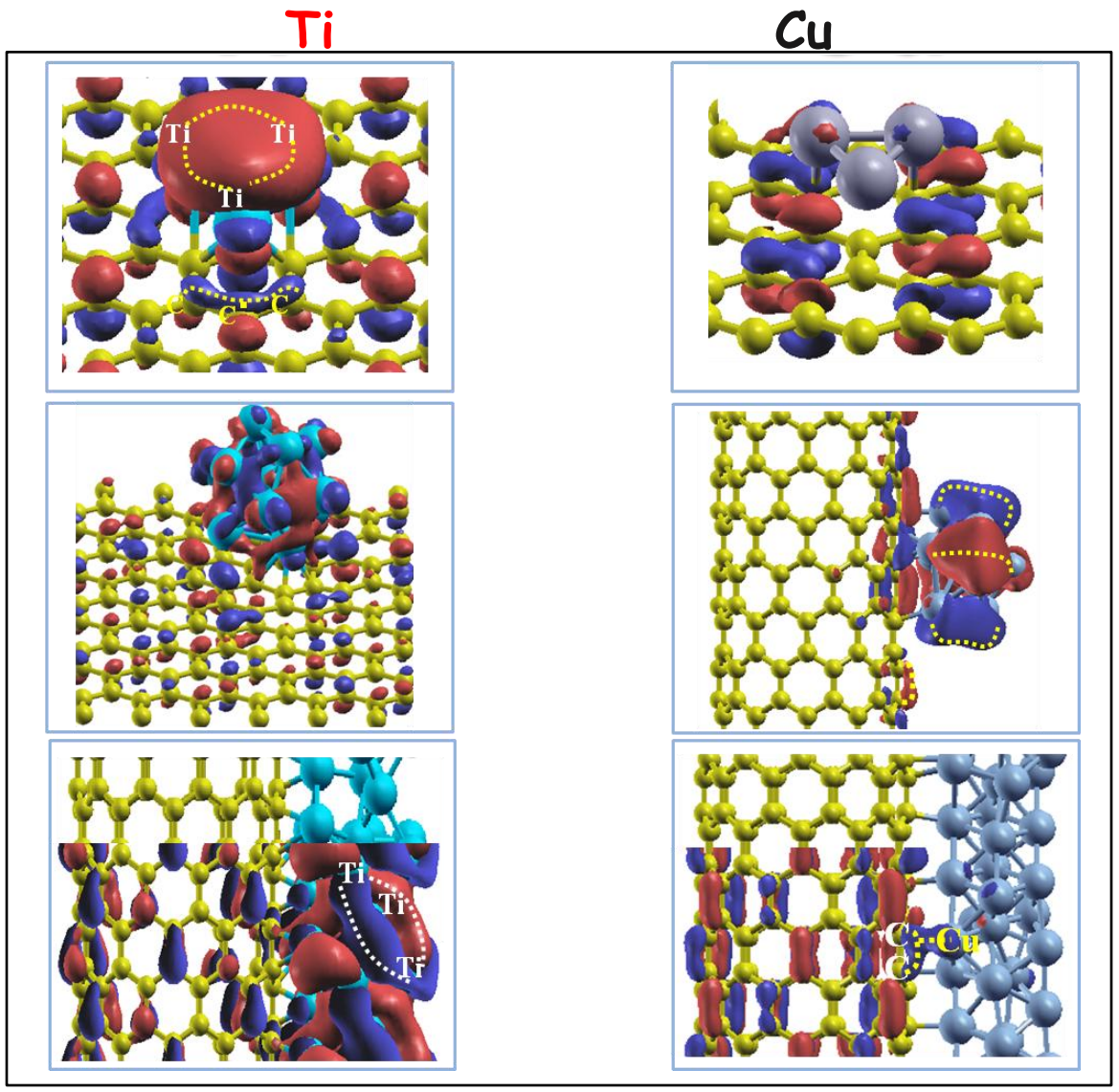


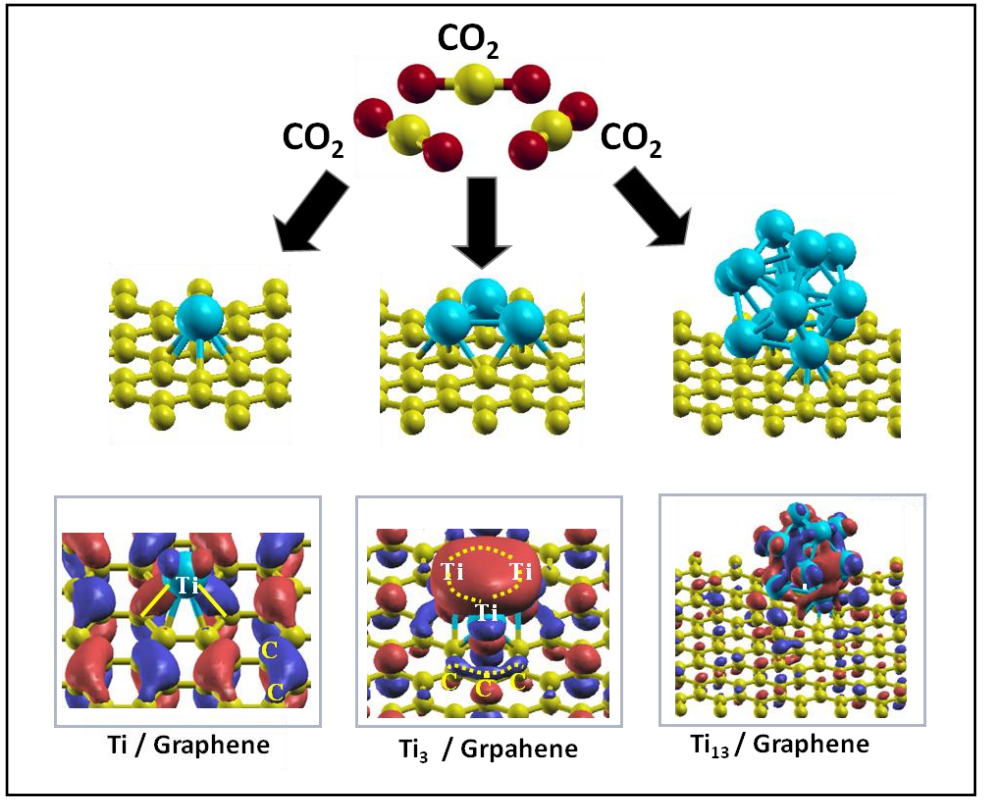
Cu

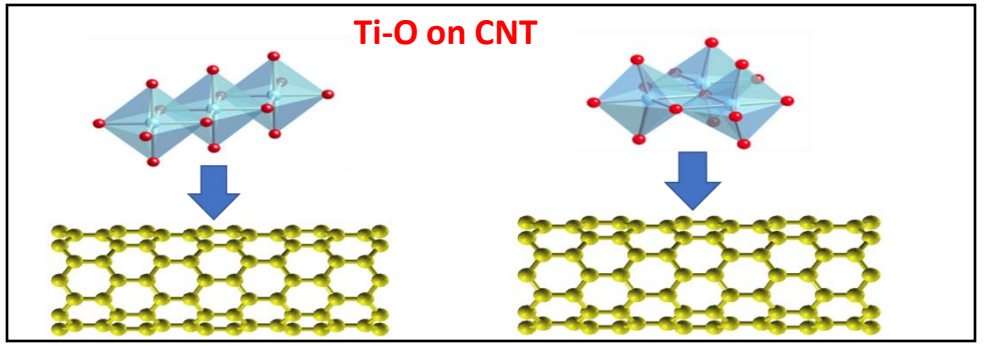


Ti_N Decoration of Single-Wall Carbon Nanotubes and Graphene by Density Functional Theory Computations,
M. A. Gialampouki and Ch. E. Lekka, J. Phys. Chem. C 115 (2011) 15172–15181,
Structural and electronic properties of Ti-nanowires/C-single wall nanotubes composites by density functional theory calculations
M.A. Gialampouki, A.V. Balerba, Ch.E. Lekka, Materials Chemistry and Physics 134 (2012) 214– 218,

Metallic Nanostructures on CNTs and Graphene



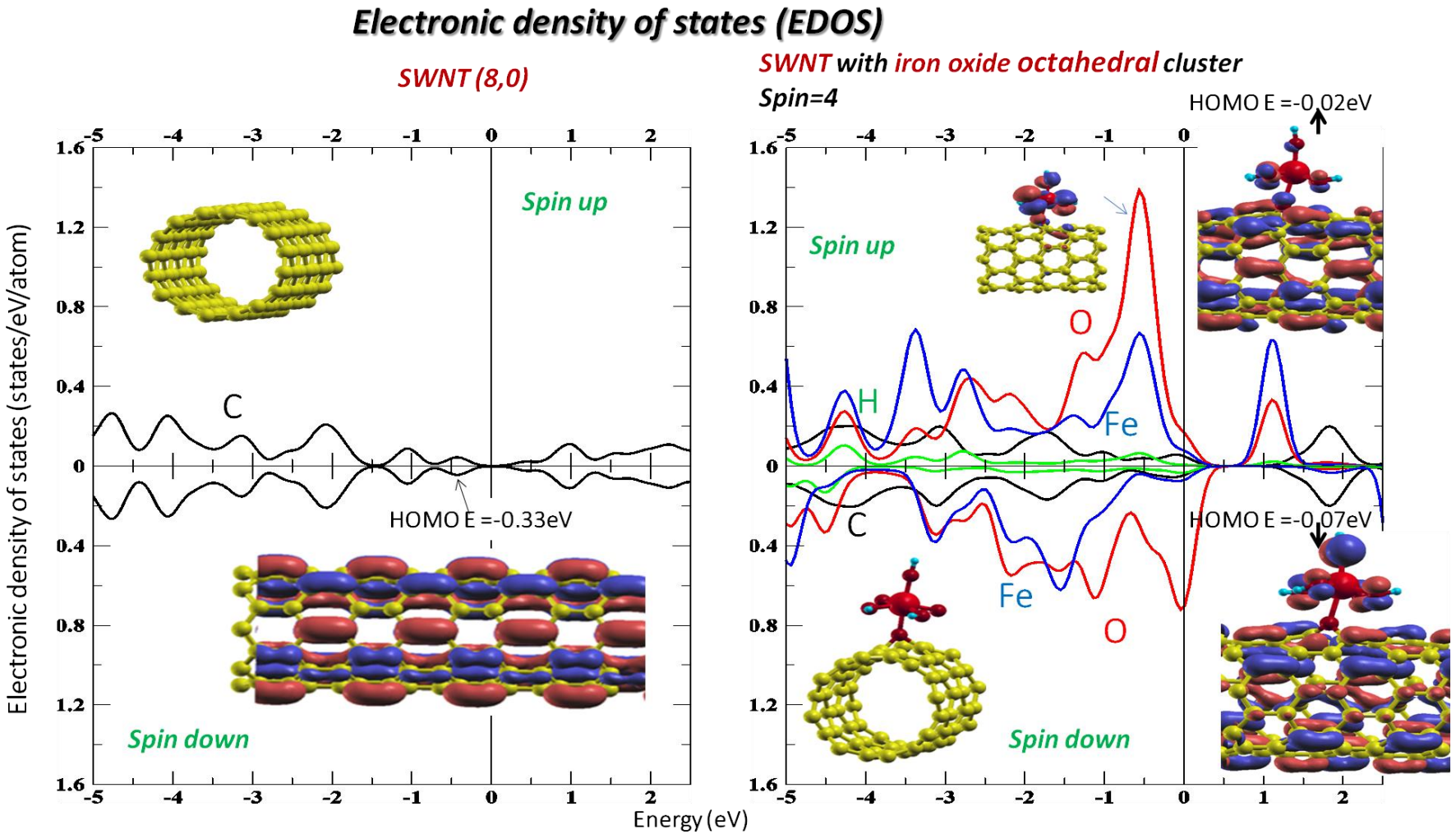




Early Stages of Ti−O Cluster Growth on Carbon Nanotubes by ab-Initio Calculations,
M. A. Gialampouki and C. E. Lekka, Journal of Physical Chemistry A, Vol.117, No.40, 10397-10406, 2013

Fe-O nanostructures on CNTs and Graphene

Controlled preparation of carbon nanotube–iron oxide nanoparticle hybrid materials by a modified wet impregnation method,
Sheodoros Tsoufis, **Alexios P. Douvalis**, Christina E. Lekka, Pantelis N. Trikalitis, **Thomas Bakas, Dimitrios Gournis**, J Nanopart Res (2013) 15:1924



Materials for environmentally sustainable applications

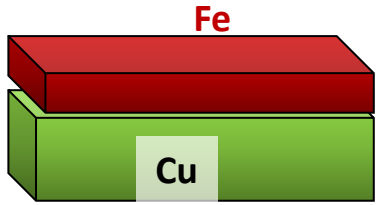
SELECTA Coordinator
Prof. J. Sort, UAB, Spain

Dr E. Pelliker,
UAB, Spain

H2020-MSCA-ITN-2014: Smart ELECTrodeposited Alloys for environmentally sustainable applications: from advanced protective coatings to micro/nano-robotic platforms

http://selecta-etn.eu/

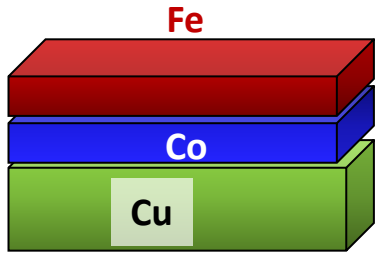
Salvador Pané et al, *European Ophthalmic Review,* 2014;8(2):120–6

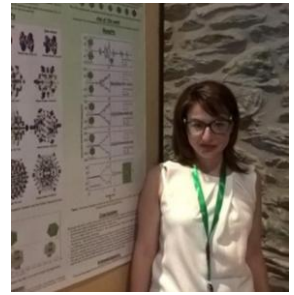


Fe coating on

Non-magnetic Cu substrate

Magnetic Co substrate





Dr C. Cutrano

Experimental studies

Fe film's structure and magnetic moment depends on its thickness

Fe / Cu(100)[1]:

Up to 5 Fe ML on Cu(100)→ Fe fct film ferromagnetic(Fe surf 2.5-2.8 μ_B), Fe_{bcc}=2.2μ_B

1. M. Donath, J. Phys. Condens. Mater 11 (1999) 9421
2. X. Yin, K. Hermann, Phys. Rev. B 63 (2001) 115417
3. H. Choi, S.G. Lee, Y.C.Chung, Comp. Mater. Scie. 49 (2010) S291

Fe / Co / Cu (100):

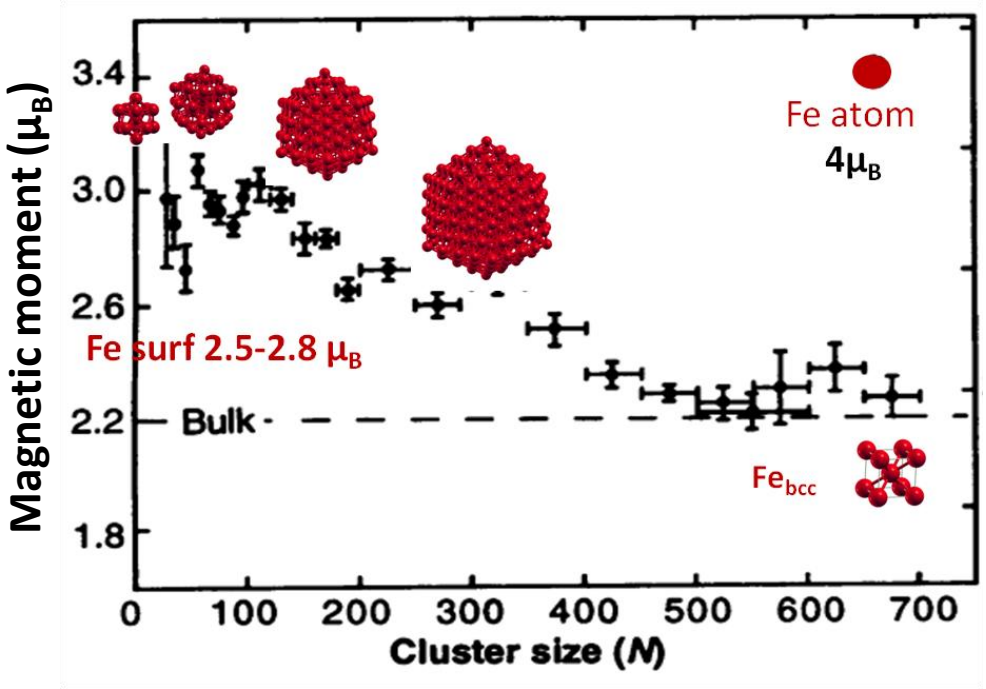
Up to 4-6 Fe ML fct film with 2-3 μ_B on Co/Cu(100)[1,2]

1. N. Kamakura, A. Kimura, T. Saitoh, O. Rader, K.S. An, A. Kakizaki, Phys. Rev. B 73 (2006) 094437
2. D. Schmitz, C.Charton, A. Scholl, C. Carbone W. Eberhardt, Phys. Rev.B 59 (1999)

Materials for environmentally sustainable applications

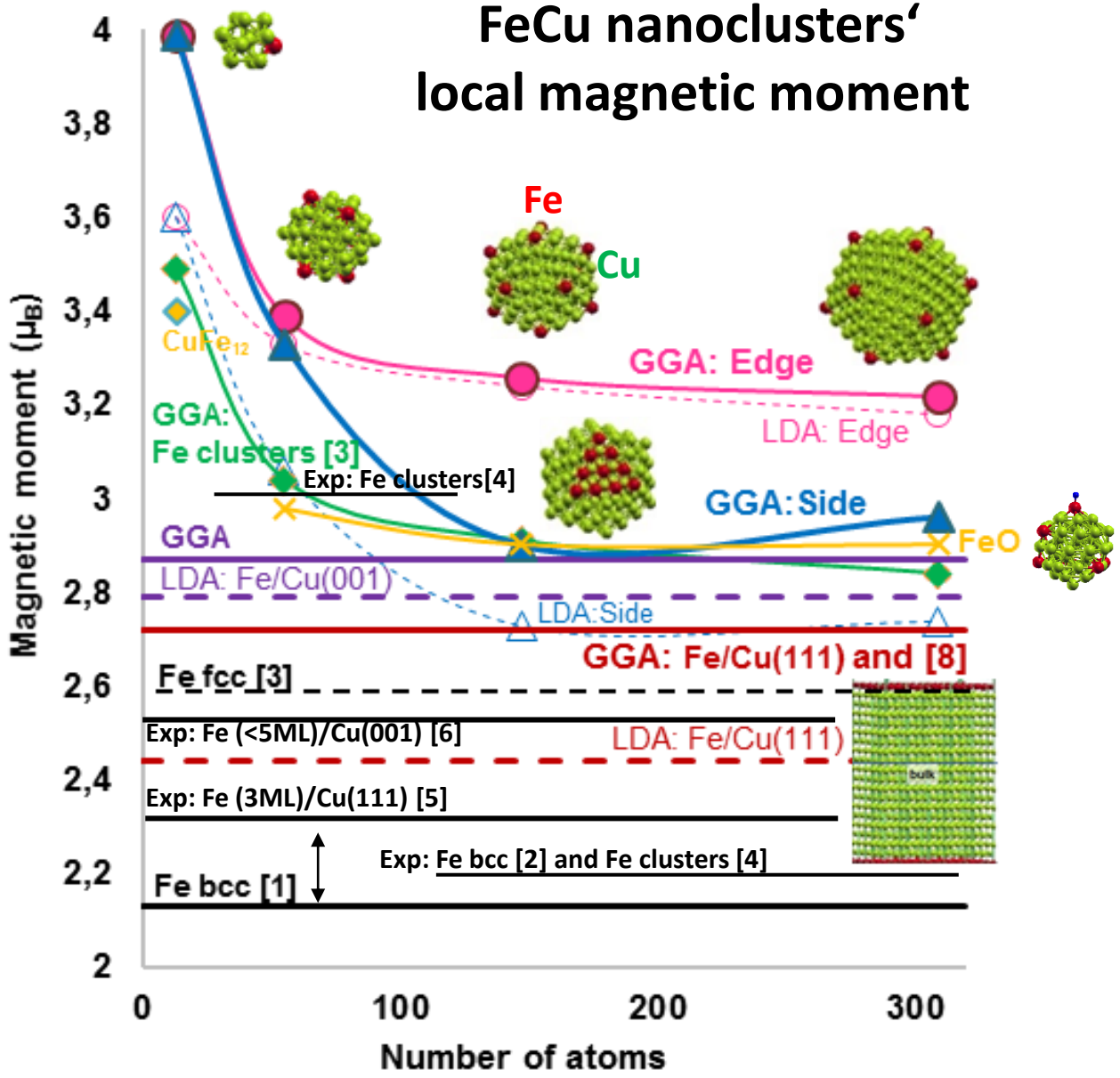
Fe nanoclusters

Experiment

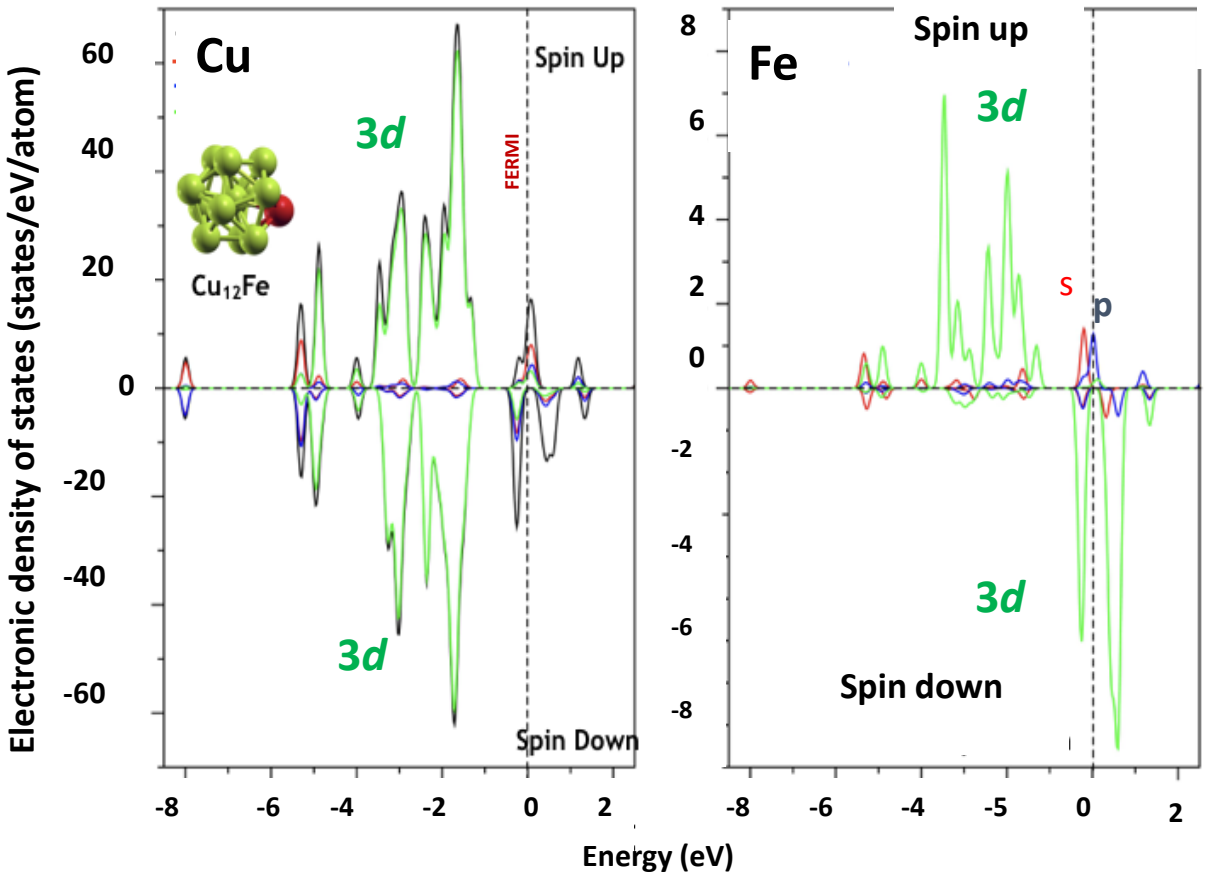


Billas I M L, Chatelain A, de Heer W A. Science. 1994; 265:1682-1684

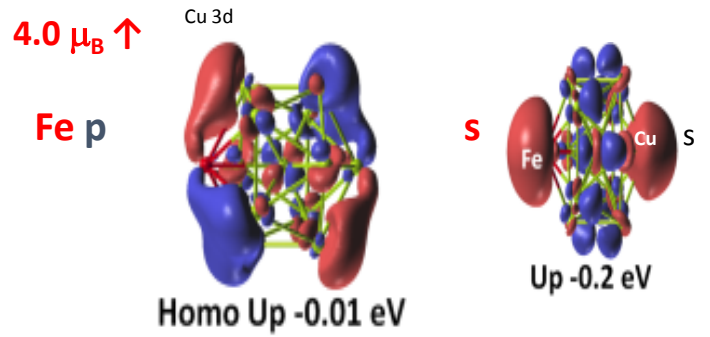
FeCu nanoclusters' local magnetic moment



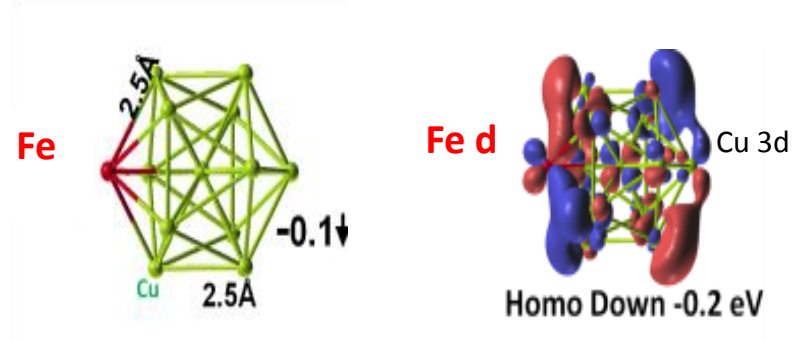
Materials for environmentally sustainable applications



Spin up : All Fe 3*d* (4.1e⁻) are occupied and *4p (2.87e⁻)*



Spin down: less Fe 3*d (1.7e⁻)* are occupied

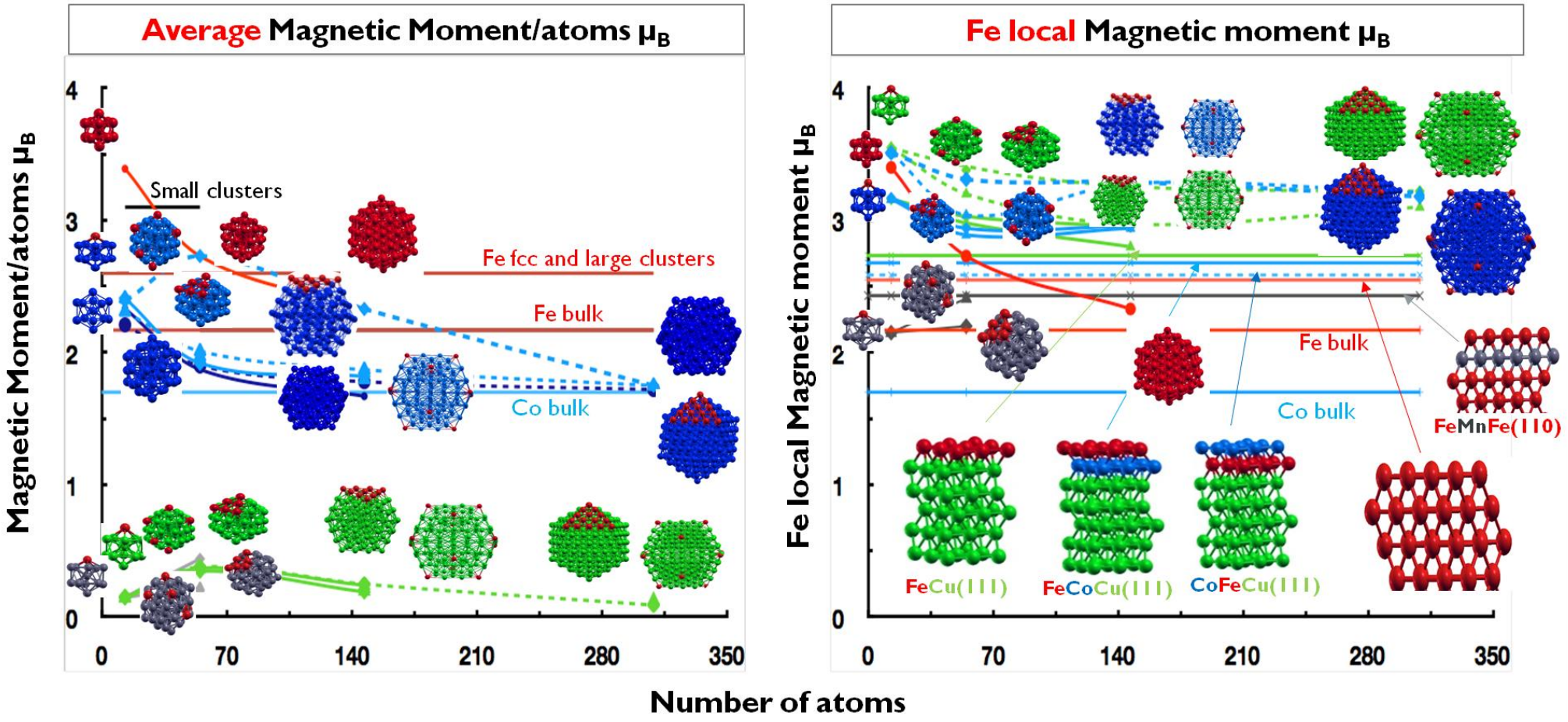


- 'Structural, magnetic and electronic properties of Cu-Fe nanoclusters by density functional theory calculations' C.S. Cutrano, Ch.E. Lekka, Journal of Alloys and Compounds 707 (2017) 114-119.
- 'Fe–Co magnetic nanoclusters by density functional theory calculations ' C.S.Cutrano,Ch.E. Lekka, Materials Science and Technology, 34 (2018) 1575-1581.

Materials for environmentally sustainable applications

Fe-X clusters and coatings

X=Cu, Co and Mn

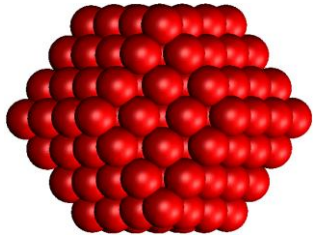


C.S. Cutrano, Ch.E. Lekka, Journal of Alloys and Compounds 707 (2017) 114-119.
C.S.Cutrano,Ch.E. Lekka, Materials Science and Technology, 34 (2018) 1575-1581

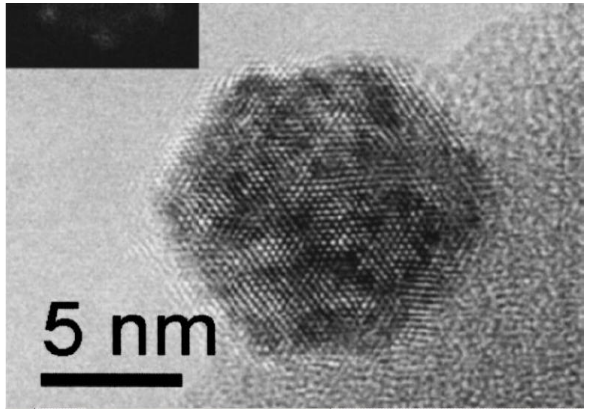
Structure and electronic properties of nano-materials

Prof
Papaconstantopoulos
U.S. Naval Res Lab

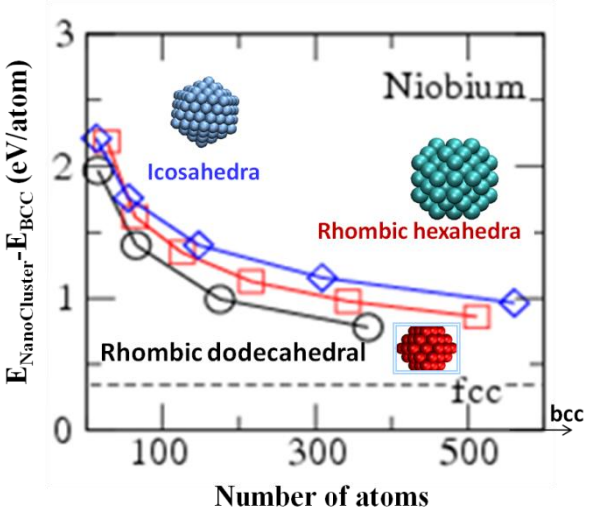
Nanoclusters

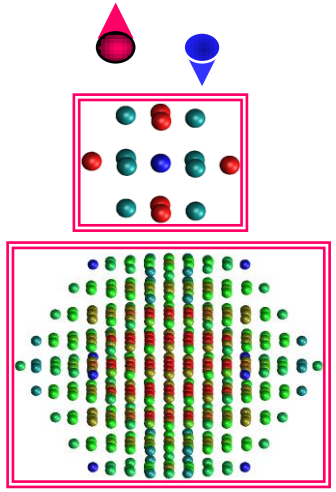


2.5nm



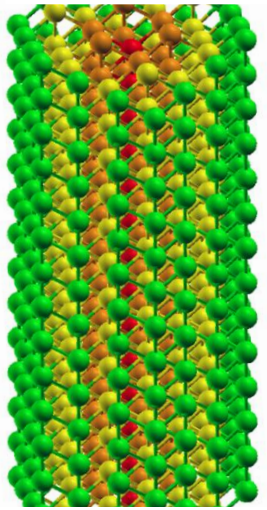
. T. Vystavel, APL 83 (2003) 3909





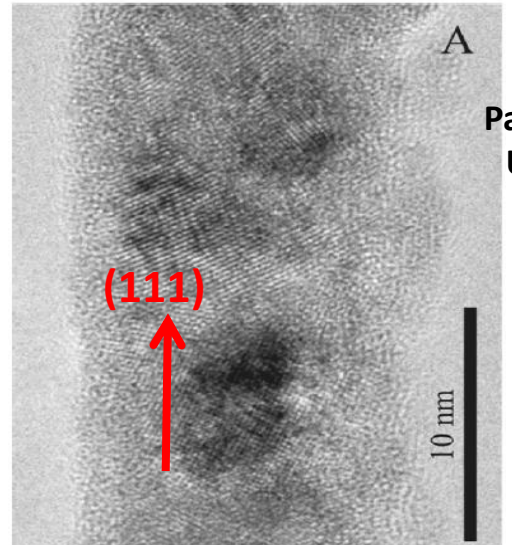
Charge transfer

Nanowires



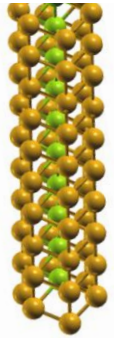
2.2nm

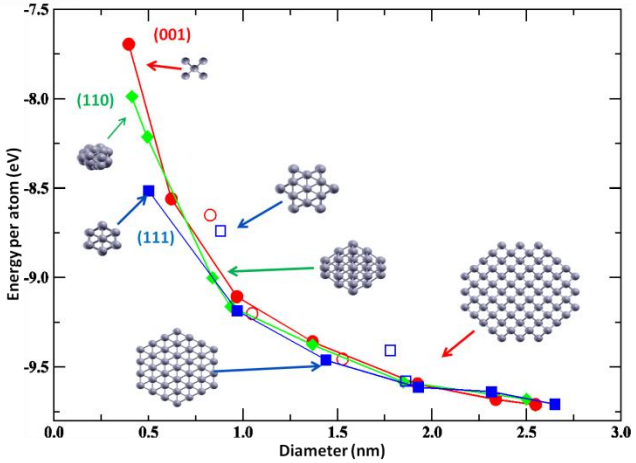
(111)



A. Rogacheva , APL83 (2003) 512

0.6nm



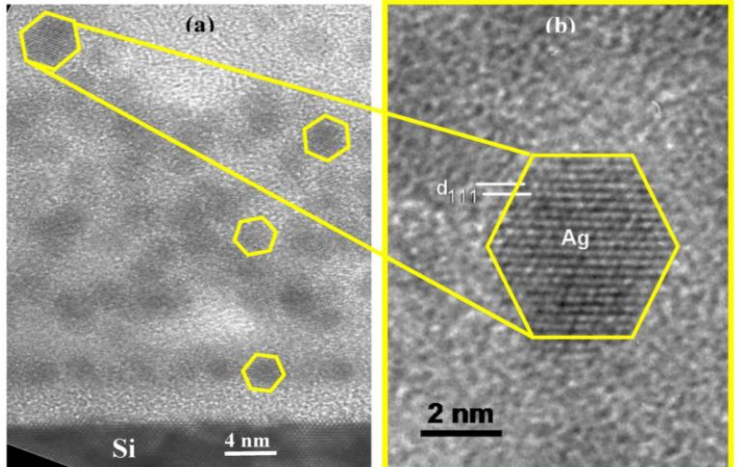


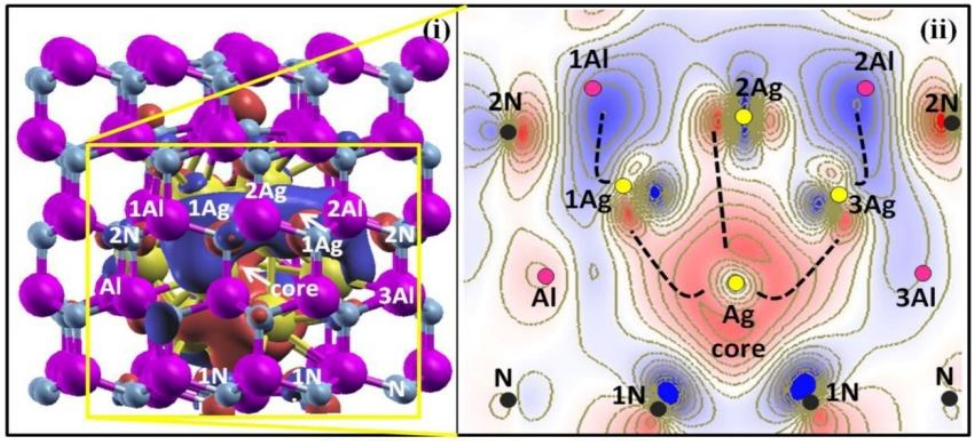
Ch.E. Lekka, M.J. Mehl, N. Bernstein, D.A. Papaconstantopoulos, Phys. Rev. B68 (2003) 35422.
Ch.E. Lekka, D.A. Papaconstantopoulos, Surface Science 601 (2007) 3937–3942

Nitrides

AlN:Ag nanocomposite film

Electronic properties and bonding characteristics of AlN:Ag thin film nanocomposites, Ch. E. Lekka, **P. Patsalas, Ph. Komninou**, and **G. A. Evangelakis,** Journal of applied physics 109 (2011) 054310-054316





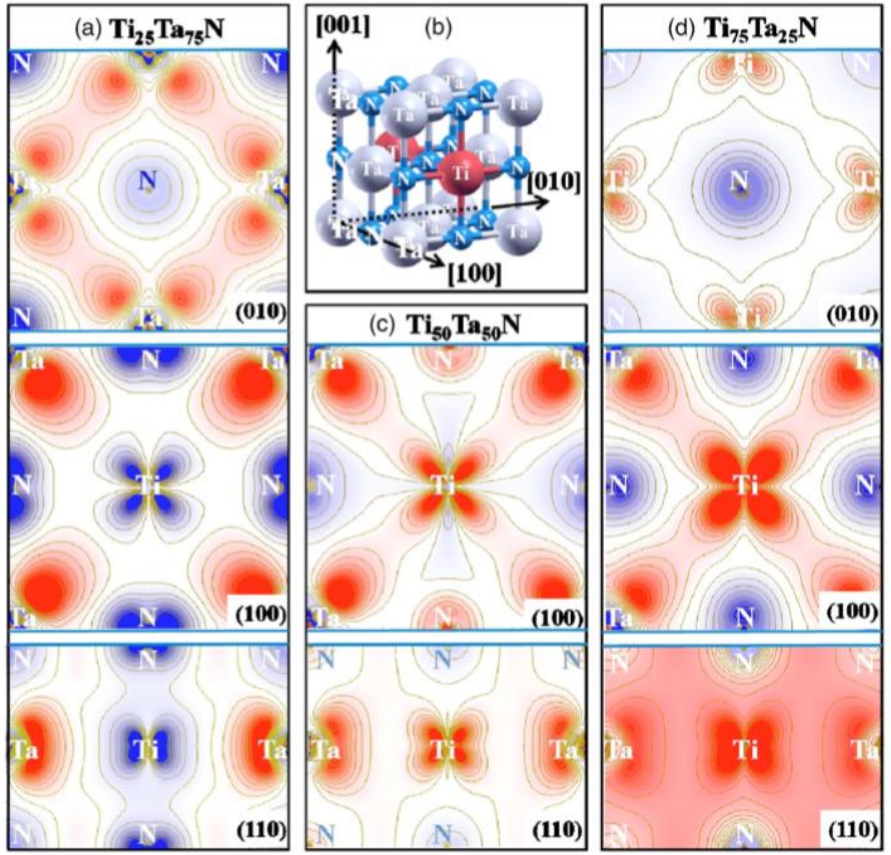
d) AlN:Ag_{13} WF at -5.6eV

Hybridization of Ag-*p* :N-*p* and Ag-*d*: Al-*p* along with charge transfer from Al → Ag

Prof. P. Patsalas

TiTaN nitrides

Conductive nitrides: Growth principles, optical and electronic properties, and their perspectives in photonics and plasmonics, **Patsalas, P.,** Kalfagiannis, N., Kassavetis, S., G.Abadias, D.V. Bellas, Lekka, **C., Lidorikis**, E., Materials Science and Engineering R: Reports, 2018, 123, pp. 1-55



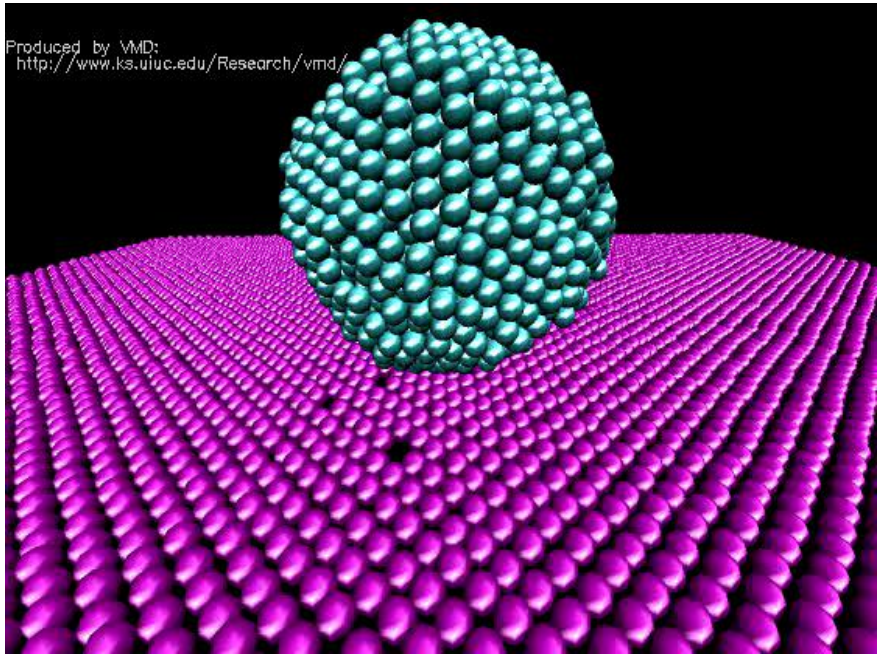
Conducting transition metal nitride thin films with tailored cell sizes: the case of δ-TixTa1-xN, L.E. Koutsokeras, G. Abadias, Ch.E. Lekka, G.M. Matenoglou, D.F. Anagnostopoulos, G.A. Evangelakis and P. Patsalas APL **93** (2008) 011904

Δομικές και μηχανικές ιδιότητες Νανο–υλικών

Δ. Παπαγεωργίου
Αναπλ. Καθηγητής

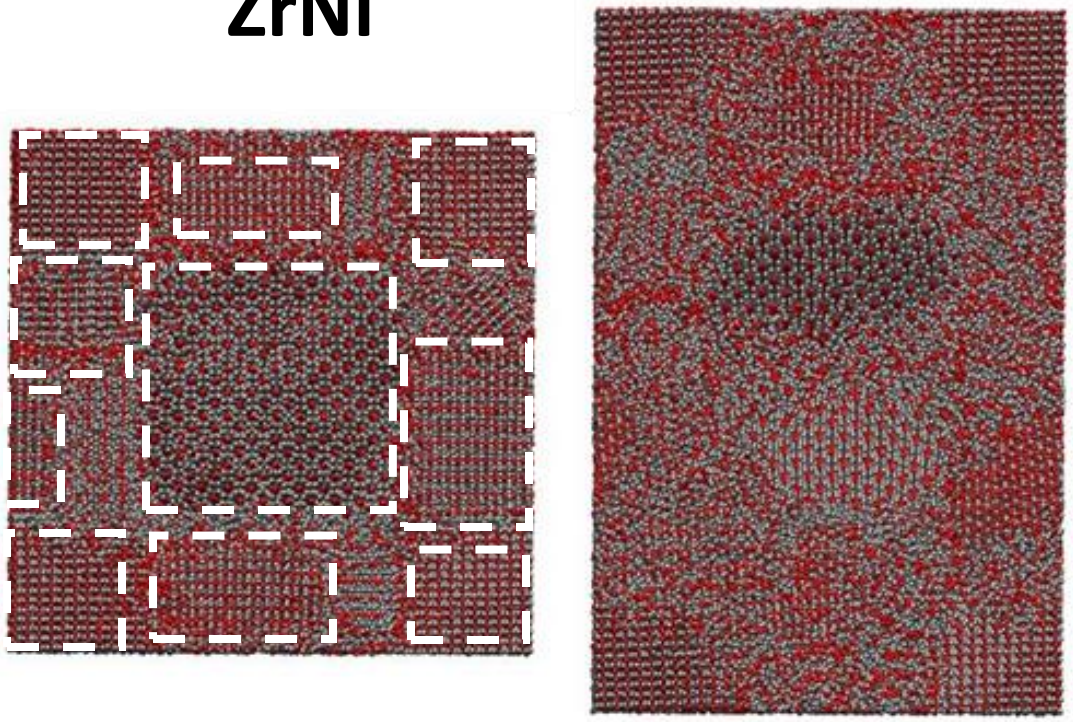
Γ. Ευαγγελάκης
Καθηγητής

Al nanoclusters on Al(111)



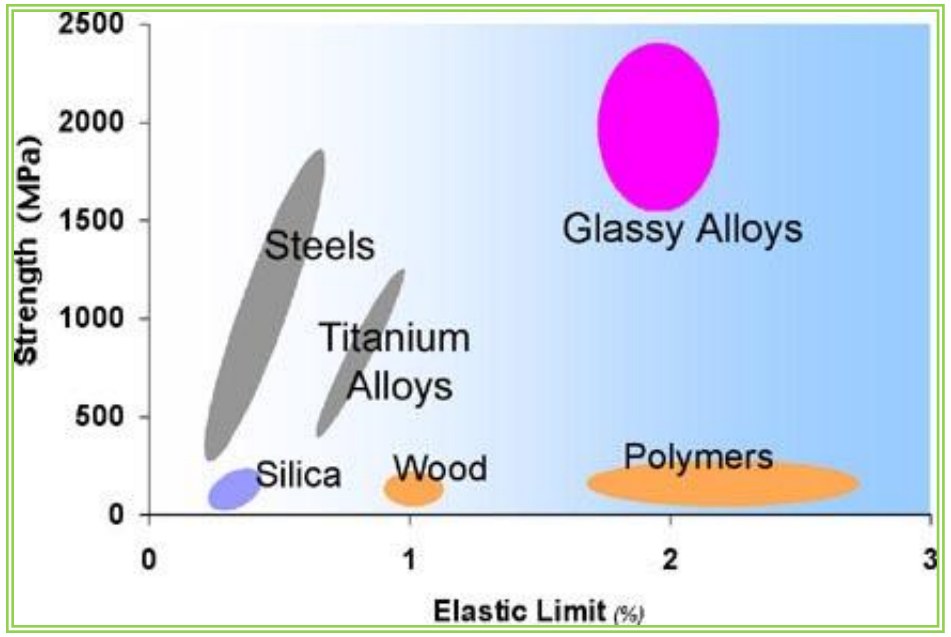
Electronic, Structural and Thermodynamic properties of icosahedral free and supported Al clusters on Al surfaces from Tight Binding and classical Molecular Dynamics simulations, P. Mitev, D.G. Papageorgiou, Ch.E. Lekka and G.A. Evangelakis, Surf.Sci. 566-568 (2004) 937

Nanoclustered ZrNi

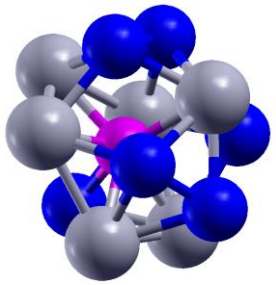


G.A. Evangelakis, D.G.Papageorgiou, Ch.E.Lekka, I.E. Lagaris, JALCOM. 434-435 (2007) 546.
A. Ibenskas, Ch.E. Lekka and G.A. Evangelakis, Physica B37 (2007) 189

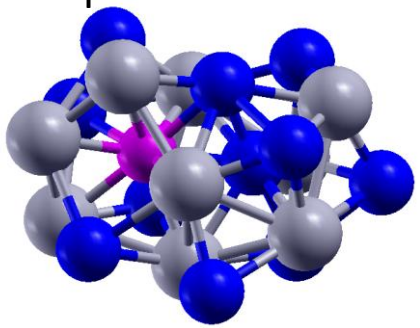
Metallic glasses: Υλικά με εξαιρετικές μηχανικές ιδιότητες



Nano-clusters



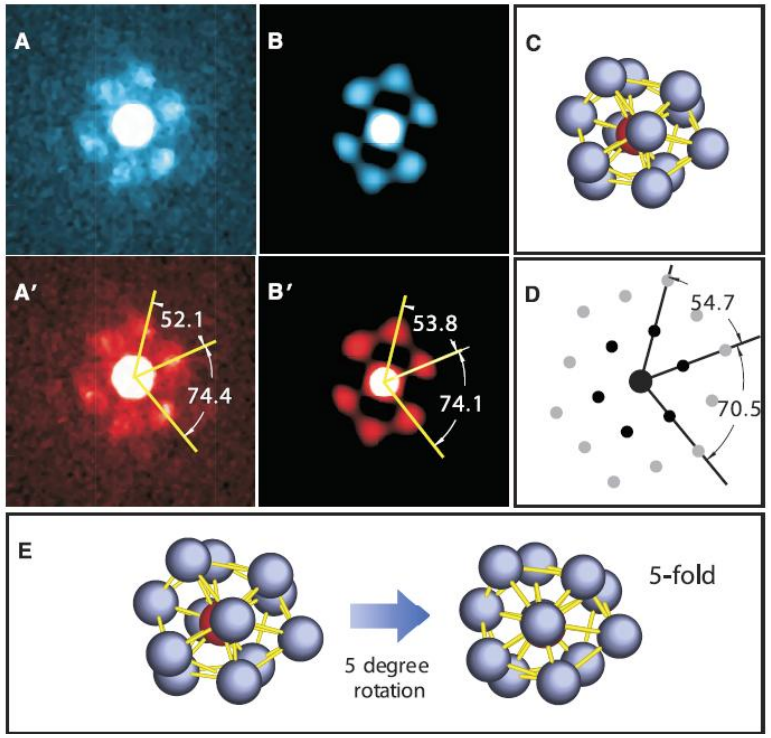
Super-Clusters



Dr G. Bokas
Γ. Μπόκας, Siemens

Δ. Παπαγεωργίου
Αναπλ. Καθηγητής

Γ. Ευαγγελάκης
Καθηγητής



Distorted icosahedron taken from fcc-like orientation
Hirata A., Kang L.J, Fujita T., Klumov B., Matsue K., Kotani M., **Yavari A.R.**, Chen M.W., **Science**, 341, **2013**, 376-9

Prof. Eckert, Leoben
Dr. N. Mattern, Prof M.Calin, Dr M. Stoica, Dr A. Gebert, IFW Dresden

Prof. R. Yavari*
Grenoble INP

FP7-PEOPLE-2013-ITN:
Vitrified Metals Technologies and Applications in
http://www.vitrimettech.unito.it/

Metallic glasses: Υλικά με εξαιρετικές μηχανικές ιδιότητες

"Work-Hardenable" Ductile Bulk Metallic Glass
J. Das et al, J. Eckert, PRL94 (2005) 205501

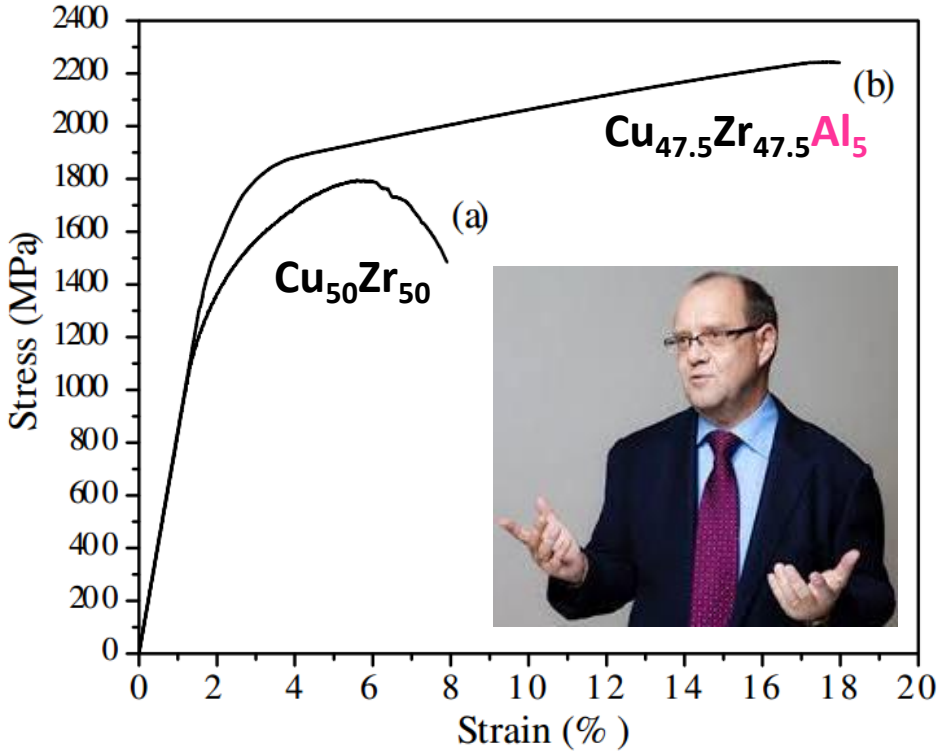
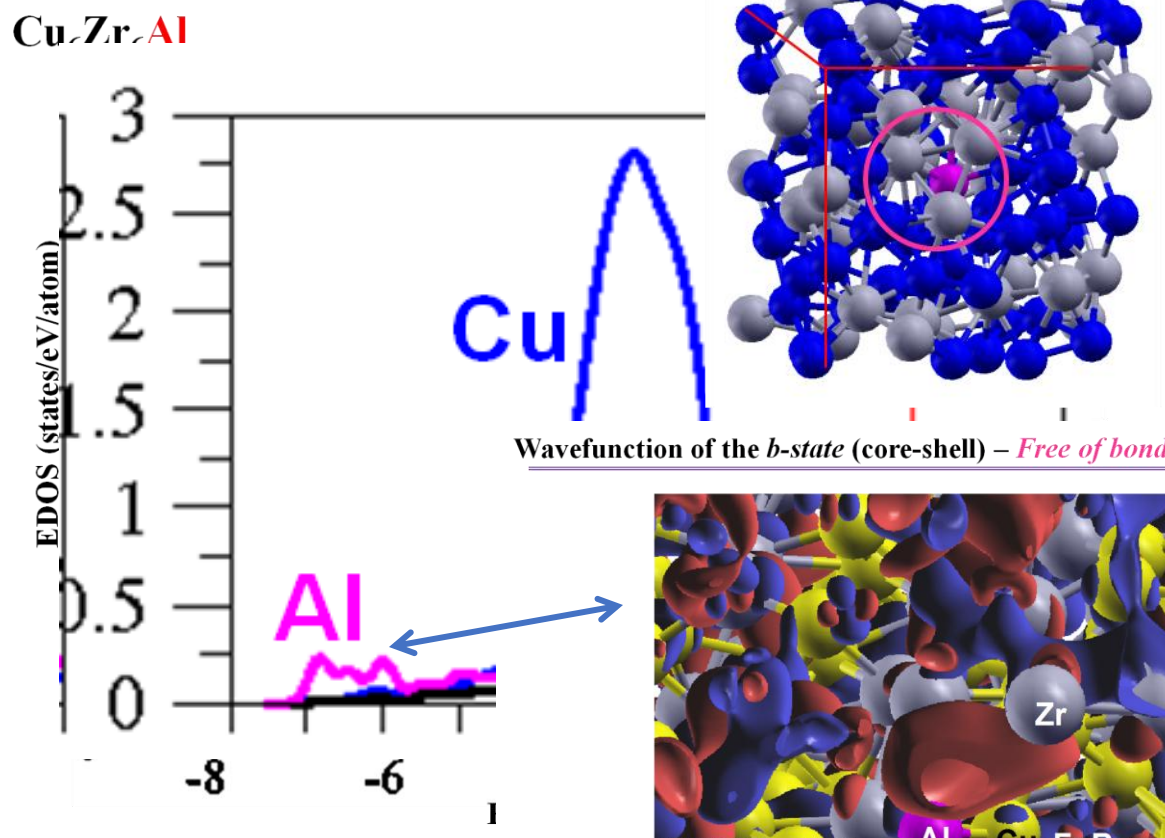


FIG. 2. Stress-strain curves of (a) $Cu_{50}Zr_{50}$ and (b) $Cu_{47.5}Zr_{47.5}Al_5$ under compression at a strain rate of $8 \times$

$Cu_{62}Zr_{37}Al$



Wavefunction of the *b-state* (core-shell) – *Free of bond plane*

Ch. E. Lekka , G.A. Evangelakis Scripta Mater.61 (2009) 974
Ch. E. Lekka JALCOM, 504 (2010) 190
G. Bokas G.A. Evangelakis , Ch. Lekka Comp. Mater. Scie. 50 (2011), 2658-2662
Ch.E.Lekka, G. Bokas, G.A.Almyras, D.G.Papageorgiou, G.A.Evangelakis, JALCOM 536 (2012) S65
G.B. Bokas , A.E. Lagogianni , G.A. Almyras , Ch.E. Lekka , D.G. Papageorgiou , G.A. Evangelakis Intermetallics 43 (2013) 138
G.B. Bokas, Ch.E. Lekka, D.G. Papageorgiou, G.A. Evangelakis, Polyhedron 133 (2017) 1–7

BioTiNet
Marie Curie Initial Training Network

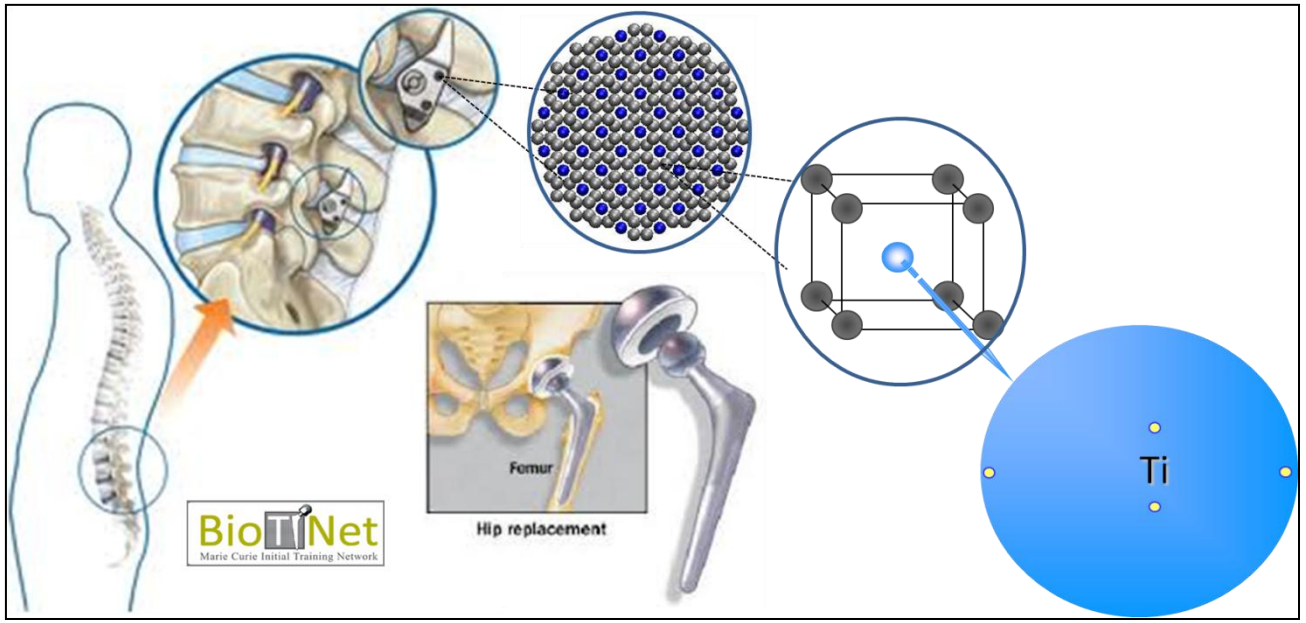
FP7-PEOPLE-2010-ITN:
Biocompatible Ti-base Structures for Orthopaedics,
http://www.biotinet.eu/

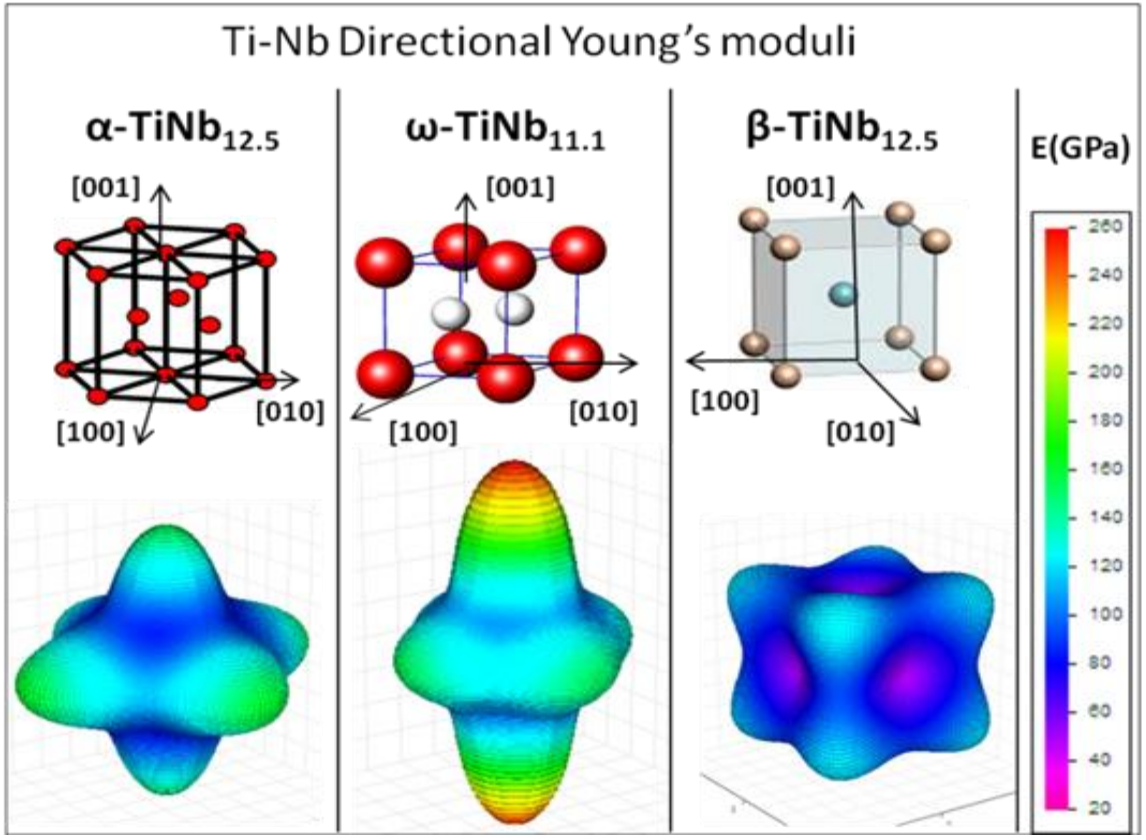
Prof. Eckert, Leoben, Austria

Prof M.Calin, Dr A. Gebert, IFW Dresden, Germany

Dr J.J.Gutierrez Moreno
BSC-CNS
Barcelona Supercomputing Center

Κράματα Ti για ορθοπεδικά : - σταθεροποίηση β-Ti μέσω **βιοσυμβατών** υλικών
- **συγκρίσιμο μέτρο ελαστικότητας** με τα **κόκκαλα**





J.J. Gutiérrez-Moreno, Ch.E. Lekka, M. Calin, J. Phys. Chem. Solids 102 (2017) 49.
Gutiérrez Moreno, J.J., Panagiotopoulos, N.T., **Evangelakis**, **G.A.**, Lekka, C.E., Materials, 2020, 13(6), pp. 1-11, 1288
J. J. Gutiérrez Moreno, **D. G. Papageorgiou,** G. A. Evangelakis, Ch. E. Lekka, J. Applied Phys. 124 (2018) 245102
Gutiérrez Moreno, J.J., Bönisch, M., Panagiotopoulos, N.T., M. Calin, D.G. Papageorgiou, A. Gebert, J. Eckert, Evangelakis, G.A., Lekka, C.E., JALCOM, 2017, 696, pp. 481-489

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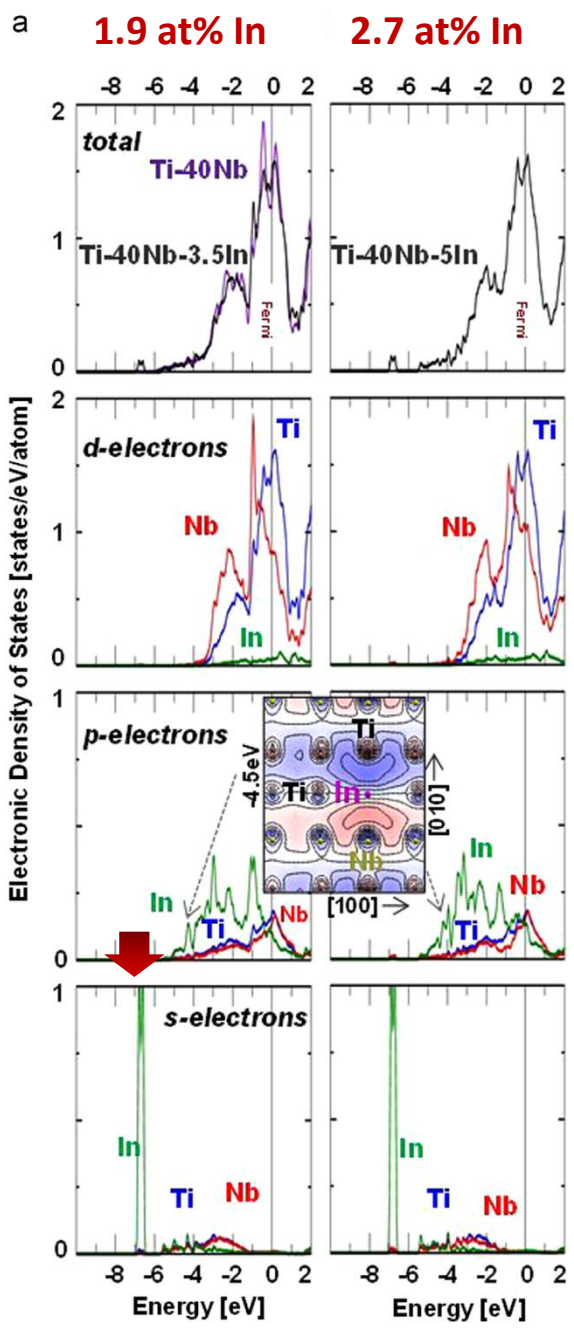
β-$TiNb_{25}In_2$

Why In or Sn decrease the β-TiNb Young moduli?

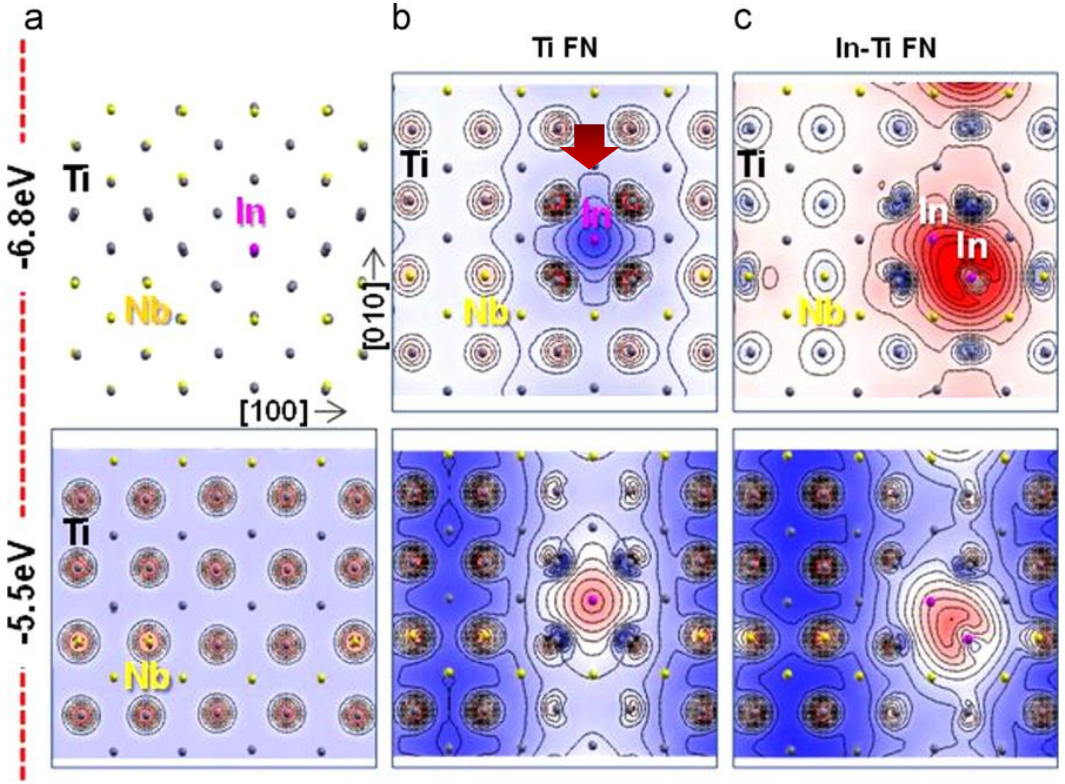
Prof. Eckert, Leoben, Austria

Prof M.Calin, Dr A. Gebert, IFW Dresden, Germany



Young moduli (GPa)

Binary β-TiNb	Ternary β-TiNbIn:	
25 at% Nb	1.9 at% In	2.7 at% In
69±0.9	51±0.5	49±0.3



Ti-In Anti-bonding states

Ti-In Anti-bonding, In-In bonding states

M. Calin, A. Helth, J. J. Gutierrez Moreno, M. Bönisch, V. Brackmann, L. Giebelera, Th. Gemming, Ch. E. Lekka, A. Gebert, R. Schnettler, J. Eckert, J. Mech. Beh. Biomed Mat 39 (2014) 162
J.J. Gutiérrez-Moreno, Y. Guo, K. Georgarakis, A.R. Yavari, G.A. Evangelakis, Ch.E. Lekka, Journal of Alloys and Compounds, JALCOM 615 (2014), S676-S679

BIOREMIA
European Training Network

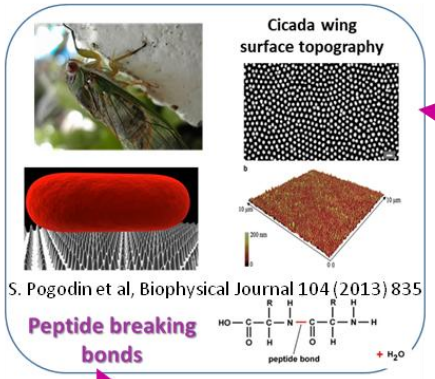
H2020-MSCA-ITN-2019, project No 861046, 2020 - 2023, BIOfilm-REsistant Materials for hard tissue Implant Applications

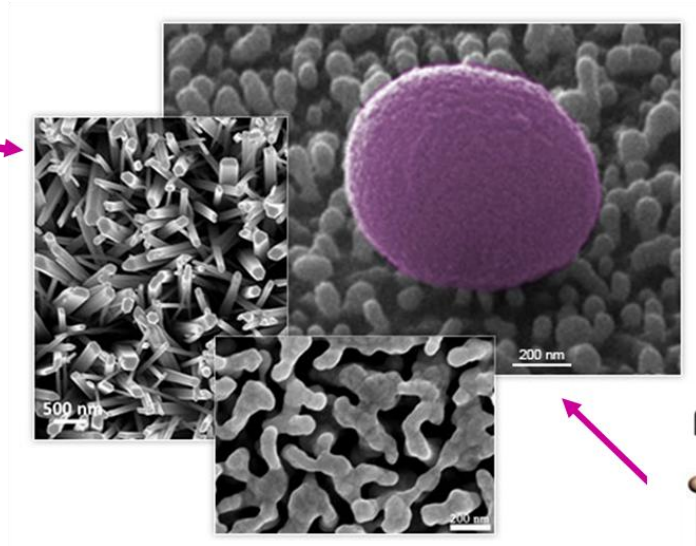

Prof M.Calin, Dr A. Gebert,
Coordinator: IFW Dresden
https://www.bioremia.eu/

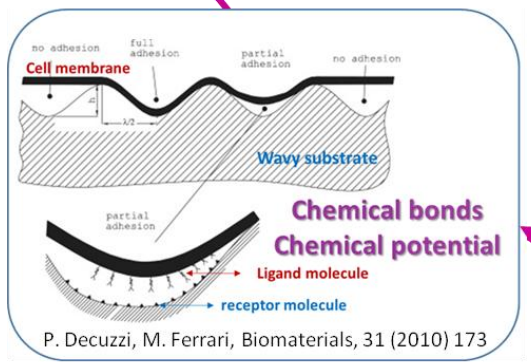
Yannick Fortouna
PhD candidate

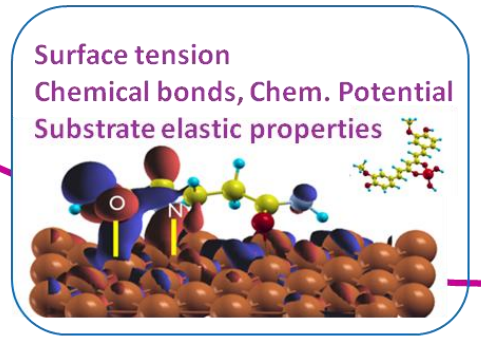
UOI-ESR1: *Antibacterial coatings of metallic surfaces:*

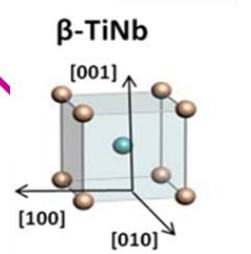
From ab-initio to large scale molecular dynamics simulations and analytical models



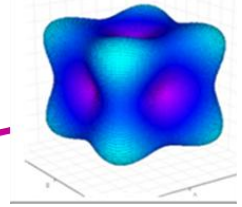








TiNb-based alloys



BIOfilm-
REsistant
Materials for hard tissue
Implant
Applications

Σας ευχαριστώ πολύ για τη προσοχή σας