

# Curriculum vitae of Ioannis N. Remediakis

**Assistant Professor, Department of Materials Science and Technology, University of Crete, Greece.**

## In short

Ioannis N. Remediakis, 42, is tenured Assistant Professor of Computational Materials Science at the Department of Materials Science and Technology, University of Crete.

He got his bachelor (1997), masters (1998) PhD (2002) degrees from the Department of Physics, University of Crete. His PhD research was performed at Harvard with Prof. Kaxiras. He had postdoc appointments with J. K. Nørskov (now at Stanford) at DTU, Denmark and P. C. Kelires (now at CUT) in Crete. He has worked as adjunct Professor (407) at Ioannina and Crete. He has payed extended visits to USC, USA and Jyvaskyla, Finland).

He employs first-principles computer simulations for low-dimensional systems, focusing on gold nanoparticles, transition metal dichalcogenides and nanocrystalline materials.

His major contribution is in the field of the atomistic Wulff construction, which is a multi-scale simulation method to predict properties of nanoparticles starting from first-principles studies of solid surfaces.

His research has been supported by EU, national and University funding, as well as several grants of CPU time in European supercomputing facilities. He has been in the management committee of two COST actions has organized two international conferences.

He teaches the main Solid-state physics/quantum physics course in both undergraduate and graduate level, as well as courses on nanoscience and simulations. He participates in various science dissemination and life-long education activities.

From 1999 to January 2018, he has 41 publications that have been cited about 2500 times according to Google Scholar. In the recent years, he has an average record of about two papers, (one every two years in journals with  $IF > 5$ ) 200 citations, two invited talks and one major seminar per year.

## Education

- 2002: PhD, Dept. of Physics, University of Crete, supervised by E. Kaxiras (Harvard) and P. C. Kelires (Crete).  
1998: MS, Condensed Matter Physics, Dept. of Physics, University of Crete.  
1997: BS, Dept. of Physics, University of Crete.

## Positions held

- 10/2014-9/2015: Head of evaluation committee, life-long education program on Materials Science (ΠΕΓΑ).  
6/2010-7/2010: Visitor, Nanotechnology center, Jyväskylä University, Finland.  
7/2009-8/2009: Visitor, Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles.  
5/2008-present: Assistant Professor, Department of Materials Science and Technology, University of Crete, Greece.  
9/2006-4/2008: Adjunct Professor (407), Department of Materials Science and Technology, University of Crete, Greece.  
9/2004-8/2006: Postdoc (supervisor: P. C. Kelires), Department of Physics, University of Crete.  
9/2002-9/2004: Postdoc (supervisor: J. K. Nørskov), Center for Atomic-scale Materials Physics, Technical University of Denmark (CAMP, DTU).  
2/2002-7/2002: Adjunct Professor (407), Department of Materials Science and Engineering, University of Ioannina, Greece.

2/1999-3/2001: Research Assistant (supervisor: E. Kaxiras), Division of Engineering and Applied Sciences, Harvard University, USA.

### **Community service**

- Member of the International organizing committee, Advances in Photocatalysis and energy materials 2017, Heraklion, 14-16/7/2017.
- Conference organizer, “Multi-Functional Nano-Carbon Composite Materials”, October 19-20, 2016, Heraklion, Crete.
- Member of the organizing committee, 30th Pan-hellenic Conference on Solid-State Physics and Materials Science, Heraklion, Crete, Sep. 2014.
- Workshop organizer, “Metal nanoparticles for advanced materials: From theory to practice”, 1-3 October, 2012, Heraklion, Crete, Greece
- Member of the organizing committee, 6th Specialist Meeting on Amorphous Carbon, Heraklion, Sep. 2006.
- Have reviewed manuscripts for the following Journals: Advanced Materials, Angewandte Chemie, Applied Catalysis, Beilstein Journal of Nanotechnology, Catalysis Letters, ChemPhysChem, Chemical Physics Letters, Chemistry of Materials, Journal of the American Chemical Society, Journal of Catalysis, Journal of Chemical Physics, Journal of Colloid and Interface Science, Journal of Physical Chemistry, Materials, Materials Science and Engineering B, Physical Review B, Physical Review Letters, Small, Solid State Electronics, Surface and Coatings Technology, Surface Science, Surface Science Reports.
- Have reviewed grant proposals for the Greek General Secretariat for Research and Technology, the German Research Foundation (DFG), the ACS Petroleum fund of USA the National Fund for Scientific Research (FNRS) of Belgium, Cy-Tera supercomputer center, and PRACE high-performance computing organization.

### **Research support and awards**

- 2017-2018: EΛΙΔΕΚ scholarship for PhD student D. Davelou.
- 2016-2020: COST Action CA15107: Multi-Functional Nano-Carbon Composite Materials Network (MultiComp). Member of the Management Committee.
- 2013- : Graphene Flagship. Member of the University of Crete group.
- 2010-2015: ERC starting grant Bio2chem-d (Grant Number: 258406, PI: Dr. N. Lopez).
- 2015: Life-Long learning program (ΠΕΓΑ: Επιστήμη Υλικών για Προηγμένες Τεχνολογίες), vice-chair (PI: K. Velonia).
- 2014-2015: Cy-tera high-performance computing grant (12 months, ca. 100000 CPU hours) after peer-review. Project: “First-principles calculations for MoS2 nanostructures”.
- 2018, 2012, 2010, 2008, 2012: Univ. of Crete Research Committee “small” and “big” programs.
- 2010-2014: COST action MP0901: “Designing novel materials for nanodevices: From Theory to Practice”. Member of the Scientific committee and Management Committee.
- 2010: HPC-Europa2 grant of CPU time in one of Europe’s largest supercomputers at Espoo,

Finland.

- 2010: HPC-Europa2 travel grant: "Surface tension of Si in the presence of volatile organic compounds".
- Best student presentation award for symposium A of EMRS Fall meeting to G. D. Barmparis, Warsaw, Poland, Sep. 2011 and to C. Motsanos in Panhellenic Conference in Solid-State Physics, Heraklion, Sep. 2008.

#### **Publications In Peer-reviewed Journals (only papers after 2005 are shown)**

1. *Ammonia synthesis from first-principles calculations*, K. Honkala, A. Hellman, I. N. Remediakis, A. Logadottir, A. Carlsson, S. Dahl, C.H. Christensen and J. K. Nørskov, *Science*, **307**, 558 (2005).
2. *\*CO oxidation on rutile-supported Au nanoparticles*, I. N. Remediakis, N. Lopez and J. K. Nørskov, *Angew. Chem. Int. Ed.* **44**, 1824 (2005).
3. *CO oxidation on gold nanoparticles: Theoretical studies*, I. N. Remediakis, N. Lopez and J. K. Nørskov, *Appl. Catal. A: General*, **291**, 13 (2005).
4. *Insights into ammonia synthesis from first principles*, A. Hellman, K. Honkala, I. N. Remediakis, A. Logadottir, A. Carlsson, S. Dahl, C.H. Christensen and J. K. Nørskov, *Surf. Sci.*, **600**, 4264 (2006).
5. *Insights into the fracture mechanisms and strength of amorphous and nanocomposite carbon*, M.G. Fyta, I.N. Remediakis, P.C. Kelires and D.A. Papaconstantopoulos, *Phys. Rev. Lett.*, **96**, 185503 (2006).
6. *Insights into the Shape and Faceting of Embedded Si/ $\alpha$ -SiO<sub>2</sub> Nanocrystals*, C. Hadjisavvas, I. N. Remediakis and P. C. Kelires, *Phys. Rev. B*, **74**, 165419 (2006).
7. *Probing the Structure and Energetics of Dislocation Cores in SiGe Alloys through Monte Carlo Simulations*, I. N. Remediakis, D. E. Jesson and P. C. Kelires, *Phys. Rev. Lett.*, **97**, 255502 (2006).
8. *Atomic and electronic structure of crystalline-amorphous carbon interfaces*, G. Kopidakis, I. N. Remediakis, M. G. Fyta and P. C. Kelires, *Diam. Rel. Mat.*, **16**, 1875 (2007).
9. *Structure, elastic properties and strength of amorphous and nanocomposite carbon*, I. N. Remediakis, M. G. Fyta, C. Mathioudakis, G. Kopidakis and P. C. Kelires, *Diam. Rel. Mat.*, **16**, 1835 (2007).
10. *Structure sensitivity of the methanation reaction: H<sub>2</sub>-induced CO dissociation on nickel surfaces*, M.P. Andersson, F. Abild-Pedersen, I.N. Remediakis, T. Bligaard, G. Jones, J. Engbæk, O. Lytken, S. Horch, J.H. Nielsen, J. Sehested, J.R. Rostrup-Nielsen, J.K. Nørskov and I. Chorkendorff, *J. Catal.* **255**, 6 (2008).
11. *Softening of ultra-nanocrystalline diamond at very small grain sizes*, I. N. Remediakis, G. Kopidakis and P. C. Kelires, *Acta Materialia*, **56**, 5340 (2008).
12. *Ammonia synthesis and decomposition on a Ru-based catalyst modeled by first-principles*, A. Hellman, K. Honkala, I. N. Remediakis, A. Logadottir, A. Carlsson, S. Dahl, C. H. Christensen, and J. K. Nørskov *Surface Science*, **603**, 1731 (2009).
13. *Mechanical Response of Nanocrystalline Materials from Atomistic Simulations*, N. V. Galanis, I. N. Remediakis and G. Kopidakis, *Physica Status Solidi*, **7**, 1372 (2010).

14. *Carbon-based nanostructured composite films: elastomechanical and optoelectronic properties from computer simulations*, M. Fyta, C. Mathioudakis, I. N. Remediakis, P. C. Kelires, *Surf. Coat. Tech.*, **206**, 696 (2011).
15. *Ordering mechanisms in epitaxial SiGe nanoislands*, G. Vantarakis, I. N. Remediakis and P. C. Kelires, *Phys. Rev. Lett.*, **108**, 176102 (2012).
16. *Dependence on CO adsorption of the shapes of multifaceted gold nanoparticles: A density functional theory*, G. D. Barmparis and I. N. Remediakis, *Phys. Rev. B* **86**, 085457 (2012).
17. *Thiolate adsorption on Au(hkl) and equilibrium shape of large thiolate-covered gold nanoparticles*, G. D. Barmparis, K. Honkala and I. N. Remediakis, *J. Chem. Phys.* **138**, 064702 (2013).
18. *Structure and mechanical properties of ultra-nanocrystalline diamond and nanocrystalline Cu from atomistic simulations*, N. V. Galanis, I. N. Remediakis and G. Kopidakis, *Mech. Mater.* **67**, 79 (2013).
19. *Silver Nanoparticles for Olefin Production: New Insights into the Mechanistic Description of Propyne Hydrogenation* G/ Vilé, D/ Baudouin, I. N. Remediakis, C. Copéret, Núria López, J. P'erez-Ramirez, *ChemCatChem*, **5**, 3750 (2013).
20. *Expanding and Reducing Complexity in Materials Science Models with Relevance in Catalysis and Energy*, K. Honkala, Z. Łodziana, I. N. Remediakis, N. Lopez, *Topics in Catalysis* **57**, 14-24 (2014).
21. *MoS<sub>2</sub> Nanostructures: Semiconductors with Metallic Edges*, D. Davelou, G. Kopidakis, G. Kioseoglou, I. N. Remediakis, Fast-track Communication, *Solid State Commun.*, **192**, 42-46 (2014).
22. *\*Nanoparticle shapes by using Wulff constructions and first-principles calculations*, G. D. Barmparis, Z. Łodziana, N. Lopez and I. N. Remediakis *Beilstein J. Nanotechn.* **6**, 361-368 (2015).
23. *Strain engineering of electronic properties of transition metal dichalcogenide monolayers*, A. E. Maniadaki, G. Kopidakis, I. N. Remediakis, *Solid State Commun.*, **227**, 33-39 (2016).
24. *Shape-Dependent Single-Electron Levels for Au Nanoparticles*, G. D. Barmparis, G. Kopidakis, I. N. Remediakis, *Materials*, **9**, 301 (2016).
25. *Shape Control in Concave Metal Nanoparticles by Etching*, Q Li, M Rellan-Pineiro, N Almora-Barrios, M Garcia-Rates, I Remediakis, N. Lopez, *Nanoscale*, **9**, 13089 (2017).
26. *Nanoribbon edges of transition-metal dichalcogenides: stability and electronic Properties*, D Davelou, G Kopidakis, E Kaxiras, IN Remediakis, *Phys. Rev. B*, **96** (16), 165436 (2017).
27. *Shape Control in Gold Nanoparticles by N-Containing Ligands: Insights from Density Functional Theory and Wulff Constructions*, M Domingo, M Shahrokhi, IN Remediakis, N Lopez, *Topics in Catalysis*, 1-7 (2018).

## Citations

According to Google Scholar (accessed Jan. 31, 2018), my publications have 2560 total citations, 1344 of which came after 2013. Hirsch index is h=20. The three most cited papers are *Science*, 307 558 (2005) (628 citations), *Angew. Chem. Int. Ed.* 44, 1824 (2005) (401 citations) and *J. Catal.*, 232, 432 (2008) (308 citations).

## Conferences

18 invited talks and 73 contributed talks/posters in international conferences/workshops, 16 seminars/colloquia at Universities and research centers. Most recent invited presentations:

1. *Introduction to modeling of materials*, invited lecturer at “Nanocomposites – characterization and properties” (summer school for advanced PhD students and postdocs), University of Białystok, Poland, 12-15/6/2017.
2. *Electronic structure of metal nanoparticles and metallic edges of 2D materials*, Towards Reality in Nanoscale Materials IX, Levi, Finland, 13-16/2/2017.
3. *Modelling the shape and properties of gold nanoparticles*, 2nd Krakow Meeting on Concepts related to Energy, Polish Academy of Sciences, Institute of Nuclear Physics, 24-25/5/2016.
4. *Shape and properties of metal nanoparticles from first-principles simulations: a multi-scale scheme* Mathematical and Computational Techniques for Molecular Systems, IACM, FORTH, Heraklion 16-18/9/15.
5. *First-principles studies of metal nanoparticles and semiconductor nanoribbons with metallic edges* AdvPhotoCat 2015, Iasi, Romania, 6-8/7/2015.
6. *Atomistic Wulff constructions for metal nanoparticles*, Israel-Greece joint meeting on nanotechnology and bionanoscience, Weizmann Institute of Science, Israel, 20-23/10/2014.
7. *Transparent transition metal oxides and chalcogenides from Density-Functional calculations: case studies*, 5th International Symposium on Transparent Conductive Materials (TCM14), Chania, 12-17/10/2014.

## Career path

1. 5/2008-: Assistant Professor, Department of Materials Science and Technology, University of Crete, Greece
  - Co-directing (with G. Kopidakis) of a research group in theoretical and computational Materials Science. The group consists of about ten researchers (group web site: <http://theory.materials.uoc.gr>).
  - Supervision of PhD theses of G. Barmparis (2012, currently in his second postdoc) “Environment-dependent shape and properties of gold nanoparticles: a first principles study”, D. Davelou (started in 2015) and D. Stefanakis (started in 2016).
  - Supervision of masters theses of P. Kotsopoulou (2014): “Theoretical study of alkanethiols adsorbed on complex gold surfaces”, D. Davelou (2015): “Theoretical and comparative study of low-dimensional transition-metal dichalcogenide structures”, A. Raptakis (2016): “Single – Electron Quantum States in Gold Nanostructures”, M. Minotakis (started in 2016), N.- R. Vrithias (started in 2016) and A. Mpoumpaki (started in 2017).
  - Supervision of diploma theses of C. Moutsanos (2010, currently self-employed): “Theoretical study of super-hard Rhenium Borides”, K. Moratis (2011, currently phd student): “Theoretical study of CaCO<sub>3</sub> allotropes”, V. Markoulaki (2013, currently Masters student), “Band-structure and optical properties of MoS<sub>2</sub> from first-principles calculations”, D. Davelou (2014): “Electronic and optical properties of one-dimensional MoS<sub>2</sub>”, M. Minotakis (2016): “Density Functional Theory Calculations For 2-D Transition Metal Dichalcogenides Alloys”.
  - Setup and teaching of four new courses in the Department: “Materials Theory” (core graduate

course, with G. Kopidakis), “Surface- and nano-science”, “Electronic Structure lab” and “Symmetry in Materials Science” (undergraduate/graduate courses); teaching of core course on Solid-State Physics.

- In collaboration with PI K. Velonia, set-up a life-long education program on materials science (ΠΕΓΑ) in 2014-2015 that run in Universities of Crete, Patras and Ioannina. IR was head of the evaluation committee, and taught several topics during the program.
- 2. 9/2006 - 4/2007: Adjunct Professor (407), Department of Materials Science and Technology, University of Crete, Greece: Teaching of core course on Solid-State Physics and elective course on “Surface- and nano-science”.
- 3. 9/2004 - 8/2006: Postdoc (in the research group of P. C. Kelires) and research fellow, Department of Physics, University of Crete: Teaching (with E. Kyritsis) of the core graduate course “Quantum Mechanics III”. Teaching (with A. Missiriotis) of the core undergraduate course on “Introduction to computer programming”.
- 4. 2/2002-7/2002: Adjunct Professor (407), Department of Materials Science and Engineering, University of Ioannina, Greece: Teaching of core course on Solid-State Physics.
- 5. 2/1999-3/2001: Research Assistant, Division of Engineering and Applied Sciences, Harvard University: Teaching assistant in the course taught by E. Kaxiras entitled “Introduction to Quantum Theory of Solids”
- 6. 7/1996 - 1/2002: Masters and PhD Student (supervisors: E. Kaxiras, P. C. Kelires), Department of Physics, University of Crete and Division of Engineering and Applied Sciences, Harvard University: Teaching assistant in several courses, including Partial Differential Equations, Solid-State Physics, Computational Physics, General Physics II, Mechanics Lab, Electromagnetism Lab, Calculus II and Modern Physics.