

# Georgios D. Barmparis

## Curriculum Vitae

### Personal Details:

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Place of Birth: Ermoupolis, Syros, Cyclades, Greece  
Citizenship: Greek  
Marital status: Engaged

### Education:

02/2008 - 09/2012 Ph.D. in Materials Science and Technology, University of Crete, Greece.  
Thesis title: "Environment-dependent shape of gold nanoparticles - a first-principles study."  
Supervisor: Ioannis N. Remediakis (University of Crete).  
2005 - 2008 M.Sc. in Computational Physics, University of Crete, Greece.  
2001 - 2005 B.Sc. in Physics with major in Computational Physics, University of Crete, Greece.  
Thesis title: "Dynamics of an impurity spin in a magnetic molecular ring."  
Supervisor: Xenophon Zotos (University of Crete).

### Research Interests

Surface chemistry (adsorption, heterogeneous catalysis), nanoscience (shape and properties of metal nanoparticles) and development of scientific software.

### Scholarships and awards

- E-MRS presentation award, E-MRS Fall Meeting (2011).
- "Maria Michail Manassaki" award as the top graduate student of the Department of Materials Science and Technology (2011).
- Individual HPC-Europa2 grant for a visit in Finland and access to one of Europe's largest computers (150000 cpu hours) (June 2010).
- IESL/FORTH scholarship for graduate studies (2007, 2008-2009).

## Publications

1. V. Markoulaki, G. D. Barmparis, G. Kioseoglou, G. Kopidakis and I. N. Remediakis, “Optical properties of single-layer MoS<sub>2</sub> under strain” (in preparation).  
*We calculate the band structure and the dielectric function of the single-layer MoS<sub>2</sub> under strain. Strain induces changes in the location of both the conduction band minimum and the valence band maximum.*
2. G. D. Barmparis, G. Kopidakis and I. N. Remediakis, “Structural and Spectroscopic Properties of Equilibrium-Shaped Au Nanoparticles” (in preparation).  
*We solve the well-known “particle-in-a-box” problem of quantum mechanics for an electron in a faceted Au nanoparticle. Electron levels can be used as an indirect probe of the interactions between Au and the encapsulating material.*
3. G. D. Barmparis, Karoliina Honkala and I. N. Remediakis, “Thiolate Adsorption on Au(*hkl*) and Equilibrium Shape of Large Thiolate-covered Gold Nanoparticles” submitted to *J. Chem. Phys.*  
*We study the dissociative chemisorption of dimethyl disulfide (CH<sub>3</sub>S–SCH<sub>3</sub>) on fourteen different Au(*hkl*), discussing trends on adsorption energies, bond lengths and bond angles as the surface structure changes. We use the results to obtain the equilibrium shape of large thiolate-covered gold nanoparticles.*
4. G. D. Barmparis and I. N. Remediakis, “A density-functional theory study on the shape of multi-faceted gold nanoparticles and its dependence on CO adsorption.” *Phys. Rev. B*, **86**, 085457 (2012).  
*We study the equilibrium shape of large clean and CO-covered gold nanoparticles, inaccessible by direct atomistic simulations. We discuss trends on adsorption of CO on several different Au surfaces. Nanoparticles become rounded and more reactive upon exposure to CO.*
5. J. S. Hummelshøj, D. D. Landis, J. Voss, T. Jiang, A. Tekin, N. Bork, M. Dułak, J. J. Mortensen, L. Adamska, J. Andersin, J. D. Baran, **G. D. Barmparis**, F. Bell, A. L. Bezanilla, J. Bjork, M. E. Björketun, F. Bleken, F. Buchter, M. Bürkle, P. D. Burton, B. B. Buus, A. Calborean, F. Calle-Vallejo, S. Casolo, B. D. Chandler, D. H. Chi, I Czekaj, S. Datta, A. Datye, A. DeLaRiva, V Despoja, S. Dobrin, M. Engelund, L. Ferrighi, P. Frondelius, Q. Fu, A. Fuentes, J. Füst, A. García-Fuente, J. Gavnholt, R. Goeke, S. Gudmundsdottir, K. D. Hammond, H. A. Hansen, D. Hibbitts, E. Hobi, Jr., J. G. Howalt, S. L. Hruby, A. Huth, L. Isaeva, J. Jelic, I. J. T. Jensen, K. A. Kacprzak, A. Kelkkanen, D. Kelsey, D. S. Kesanakurthi, J. Kleis, P. J. Klüpfel, I Konstantinov, R. Korytar, P. Koskinen, C. Krishna, E. Kunkes, A. H. Larsen, J. M. G. Lastra, H. Lin, O. Lopez-Acevedo, M. Mantega, J. I. Martínez, I. N. Mesa, D. J. Mowbray, J. S. G. Mýrdal, Y. Natanzon, A. Nistor, T. Olsen, H. Park, L. S. Pedroza, V Petzold, C. Plaisance, J. A. Rasmussen, H. Ren, M. Rizzi, A. S. Ronco, C. Rostgaard, S. Saadi, L. A. Salguero, E. J. G. Santos, A. L. Schoenhalz, J. Shen, M. Smedemand, O. J. Stausholm-Møller, M. Stibius, M. Strange, H. B. Su, B. Temel, A. Toftelund, V Tripkovic, M. Vanin, V Viswanathan, A. Vojvodic, S. Wang, J. Wellendorff, K. S. Thygesen, J. Rossmeisl, T. Bligaard, K. W. Jacobsen, J. K. Nørskov and T. Vegge “Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project.” *J. Chem. Phys.* **131** (1): 014101 (2009).  
*We investigate the stability and decomposition of alloys containing 1 alkali metal atom, Li, Na, or K (M<sub>1</sub>); and 1 alkali, alkaline earth or 3d/4d transition metal atom (M<sub>2</sub>) plus two to five (BH<sub>4</sub>)<sup>−</sup> groups, using a number of model structures with trigonal, tetrahedral, octahedral, and free coordination of the metal borohydride complexes. This work was performed during the 2008 CAMD Summer School in “Electronic Structure Theory and Materials Design”, Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark.*

Reprints of papers can be found at <http://theory.materials.uoc.gr/people/barmparis/> .

## Other publications

1. “*Environment-dependent shape of gold nanoparticles - a first-principles study*”, Georgios D. Barmparis, Ph.D. Thesis, Department of Materials Science and Technology, University of Crete, 2012 (in preparation).
2. “*Equilibrium Shape of Thiolate-Covered Au Nanoparticles. A virtual laboratory for nanoparticle synthesis*”, HPC-Europa2 newsletter “Science and Supercomputing in Europe - research highlights 2010”.

## Conferences - Summer Schools

1. “*Surface chemistry of gold and the equilibrium shape of Au nanoparticles from first-principles simulations*”, XXVIII Panhellenic Conference on Solid State Physics and Materials Science, University of Patras, Patra, Greece, 23-26 September, 2012 (will be presented by I. N. Remediakis, invited talk).
2. “*First-principles study of adsorption on Au(hkl) and the shape of gold nanoparticles*”, E-MRS 2012 Fall Meeting, Warsaw University of Technology, Poland, 17-21 September, 2012.
3. “*Optical properties of single-layer MoS<sub>2</sub> under strain*”, E-MRS 2012 Fall Meeting, Warsaw University of Technology, Poland, 17-21 September, 2012 (will be presented by I. N. Remediakis).
4. “*First-principles study of adsorption on Au(hkl) and the shape of gold nanoparticles*”, Quantum-chemical modelling of large nanostructures, Aveiro, Portugal, 6-9 June, 2012 (presented by I. N. Remediakis, invited talk).
5. “*Equilibrium shape of gold nanoparticles*”, Designing novel materials for nanodevices: From Theory to Practice (NanoTP), Trieste, Italy, 9-11 November, 2011 (presented by I. N. Remediakis).
6. “*Shape changes of Au nanoparticles in reactive environment*”, E-MRS 2011 Fall Meeting, Warsaw University of Technology, Poland, 19-23 September, 2011 (presentation award).
7. “*Shape changes of Au nanoparticles in reactive environment*”, DFT 2011, 14<sup>th</sup> International Density Functional Theory Conference. Applications in Physics, Chemistry, Biology, Pharmacy, Athens, Greece, 29 August - 2 September, 2011.
8. “*Equilibrium shape of Au nanoparticles from first-principles simulations*”, Vibrational Spectroscopy in Nanotechnology, Istanbul, Turkey, 26-29 June, 2011 (presented by I. N. Remediakis, invited talk).
9. “*Shape changes of Au nanoparticles in reactive environment*”, TAM 2011 Annual HPC-Europa event, Barcelona, Spain, 8-9 June, 2011.
10. “*Shape changes of Au nanoparticles in reactive environment*”, Towards Reality in Nanoscale Materials 2010 (TRNM 2010) Levi, Lapland, Finland, 6-8 December, 2010.
11. “*First-principles studies of Au nanoparticles*”, X International Conference on “Nanostructured Materials” (NANO 2010) , Rome, 13-17 September, 2010.
12. “*Equilibrium shape of nanoparticles*”, E-MRS 2011 Fall Meeting, Warsaw, Poland, 13-17 September, 2010 (presented by I. N. Remediakis).
13. “*Equilibrium shape of gold nanoparticles*”, Designing novel materials for nanodevices: From Theory to Practice (NanoTP), Berlin, Germany, 18-19 March, 2010 (presented by I. N. Remediakis).

14. *“Shape and properties of gold nanoparticles”*, Towards Reality in Nanoscale Materials 09, Levi, Finland, (7-9 December, 2009) (presented by I. N. Remediakis).
15. *“Equilibrium Shape of Gold Nanoparticles”*, 6<sup>th</sup> International Conference on Nanosciences and Nanotechnologies (NN09), Thessaloniki, Greece, 13-15 July, 2009.
16. *“Environment-dependent shape of Au nanoparticles”*, XXIV Panhellenic Conference on Solid State Physics and Materials Science, Crete, 21-24 September, 2008.
17. *“Environment-dependent shape of Au nanoparticles”*, Summer School in “Electronic Structure Theory and Materials Design”, Center of Atomic-scale Materials Design (CAMD), Physics Department, Technical University of Denmark (DTU), Copenhagen, Denmark, August, 2008.
18. Summer School in Advanced Physics, Department of Physics, University of Crete, Crete, Greece (2004, 2005, 2007).

## Teaching Experience

Teaching Assistant:

Materials Science and Technology Department, University of Crete:

2011	Fall	Laboratory Physics I: Mechanics and Heat.
2010	Fall	Laboratory Physics I: Mechanics and Heat.
2009	Fall	Solid State Physics, Introduction.
2008	Fall	Solid State Physics, Introduction.
2007	Spring	Numerical Analysis and Programming in Fortran 77.
2007	Fall	Solid State Physics, Introduction.

Physics Department, University of Crete:

2007	Spring	Numerical Analysis and Programming in Fortran 77.
2006	Spring	Numerical Analysis and Programming in Fortran 77.
2006	Fall	Programming in Fortran 77.

## Skills

Languages: Greek; English.

Operating Systems: Mac-OS X, Linux and Microsoft Windows.

Programming Languages: Fortran 77/90 (Excellent).

Python (Excellent).

Java (Excellent).

L<sup>A</sup>T<sub>E</sub>X(Excellent).

HTML (Basic).

Parallel Programming (MPI) (Basic).

Object-Oriented Techniques: Object Oriented Analysis and Design, Design Patterns, UML.

Application Packages: Dacapo, GPAW, ASAP, ASE.

## Other Activities

Founding member and first Chairman of the Postgraduate Student Association of the Department of Materials Science and Technology of the University of Crete.