Riccarda Caputo, PhD

Via Arturo Calza 37, 00157 Rome, Italy
+39 351 529 98 52 (Italy)
Nationality: Italian
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R&D Materials Scientist
Computational materials chemistry

Research expertise in first-principles computational modeling of compounds for targeted applications. IT skilled in managing large data sets and workflow of computational chemistry calculations on HPC clusters. Proactive and team-oriented senior scientist with hands-on experience in professional project management from initiation to execution, reporting and leading collaborations.

Career Highlights

- ◊ Successfully shown via computation the feasibility of theoretically predicted compounds for energy applications: hydrogen storage, batteries, solar cells compounds.
- ◊ Authored Swiss and international competitive grants and projects on theory and computation in materials design, from the idea development to computational task implementation, and leading cross-functional and international collaborations.
- ◊ Managed collaborations with industrial, experimental and theoretical groups, with the role to coach the research activity of experimental work of PhD students at ETH, EMPA and different external universities.

Areas of qualification

Crystal structure	First-principles crystal structure prediction and polymorphism of compounds, nanoparticle formation, layered compounds.
Materials by design	Structure and thermodynamic study of solid state phase formation of binary systems. Thermodynamic, electronic and dynamical properties of compounds and their dependence on structure-composition relationships.
Reactivity	Computational thermal decomposition processes in metal-organic molecules to form metallic nanoparticles, and in complex hydrides to release hydrogen.
Surface processes	Computational chemistry of surface processes in surface functionalization, adsorption and chemisorption gas/solid surface reactions.

Knowledge and Expertise

Chemistry codes	Materials Studio, CASTEP, QuantumEspresso, CPMD, phase diagram calculations, AIRSS, Turbomole, Schrödinger Materials Suite, CCDC, USPEX, GRACE (CSP).
Softwares	Shell and Vim scripting, Python, Latex, Bibtex, Gimp, Knime, Data analysis, Text mining, Office package, chemical toolkits and scientific pipelining tools.
Management	Research project, Data and literature management, Intellectual Property.
Communication	Science communication and presentation.
Publishing	Expertise in both editing and proofreading. Reviewer of different chemistry and materials chemistry journals.

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Career Development

2018-present	High-end Foreign Expert, ICQMS, Shanghai University, Department of Physics, China *Lectures and collaborative projects in computational materials modelling.*
2017-2018	Research scientist, BNF University of Bern, Switzerland Projects with Prof Adem Tekin, Technical University of Istanbul, Informatics Institute, Turkey and Prof. H. Mishra, KAUST, InterfacialLab, Saudi Arabia
2015–2016	Program Manager, EPFL NCCR *MARVEL*, Lausanne, Switzerland. *Scientific, communication and financial management of the NCCR.*
2010–2015	Research Scientist, ETH Department of Chemistry and Applied Biosciences, Zürich, Switzerland. *First principles crystal structure and property prediction of compounds for energy applications.* SCCER H&E: *Computational study of compounds for Li- and Na-battery electrodes.* SNSF Sinergia project: *Theory and modeling of metal borocarbides and metal fullerides for energy applications.*
2007–2010	Research Scientist, EMPA Division Hydrogen & Energy, Dübendorf, Switzerland. MCRTN-Hydrogen project and EMPA projects. *First-principles modeling of materials for hydrogen storage.*
2006–2007	Research Scientist, Ruhr-Universität, Department of Chemistry, Bochum, Germany. *Ab-initio calculations of adsorption reaction of benzene, CO and rare gases on noble metal surfaces using wave-functions cluster approach. Weak adsorption interactions and correlation energy contribution to adsorption energy.*
2005–2006	Research Scientist, Max-Planck Institute for Polymer Research, Mainz, Germany. *Density functional theory calculations of molecules adsorbed on transition metal surfaces as the first step to multiscale modeling. Thiols chemisorption on noble metals.*
2003	Teaching Assistant, General Inorganic Chemistry, University of Rome *La Sapienza*, Department of Geology, Rome, Italy.
2001	Teaching Assistant, General Physics, University of Rome *La Sapienza*, Department of Informatics, Rome, Italy.

Education

2005	PhD Materials Science, University of Rome *La Sapienza*, Department of Chemistry Thesis title: Hydrogen in Metals: from theory to experiments (28.02.2005).
1994	M. Sc. Chemistry, University of Rome *La Sapienza*, Department of Chemistry Thesis title: Confinamento elettrochimico di deuterio in palladio (14.07.1994, summa cum laude and thesis prize).
1987	Diploma di maturita' scientifica, Liceo Scientifico *A. Volta*, Foggia, Italy (60/60).

Other information

Languages	Italian (mother tongue), English (fluent), German (basic), French (beginner).
Award	Premio di laurea (M.Sc thesis prize) Esso-ATI Italiana, March 08 1995, Rome.
Affiliations	Editorial board Jacobs, Journal of Inorganic Chemistry (since 2016). Swiss Chemical Society (2010–2015). Swiss Chemical Society for Crystallography (2010–2015). American Chemical Society (2014).
Interests	Drawing, writing, classical music.

Scientific contributions

Publications, Conference presentations, Projects, Collaborations

Riccarda Caputo, M.Sc. Chemistry, PhD Materials Science

AREAS OF QUALIFICATION

Research & Development of Materials via first-principles methodologies.
Crystal structure prediction of molecular compounds and inorganic materials for targeted applications; structure-composition-properties relationships; thermodynamic, electronic and dynamical properties of compounds; research project management.

Publications

Papers (34) published on peer-reviewed journals, (1) under revision and (3) to be submitted.

Contributions to Conference proceedings are not listed.

Ab-initio Crystal Structure Prediction (CSP)

R. Caputo*, A. Tekin, R. Nesper
Topochemical Path in High Lithiation of MoS_2
Z. Anorg. Allg. Chem., **645**, 309-316 (2019)

Y. Liu, S. Hu, R. Caputo, K. Sun, Y. Li, G. Zhao, W. Ren
Allotropes of tellurium from first-principles crystal structure prediction calculations under pressure
RSC Adv. **8**, 39650-39656 (2018)

R. Caputo*, A. Tekin
Can lithium form phases with molybdenum?
J. Solid State Chem., **271**, 230-238 (2019)

N. Jalarvo, R. Caputo*, Y. Mettan, and T. Chatterji*
Quasielastic neutron scattering and first-principles study of the hydrogen dynamics in $H_2V_3O_8$ (under revision)

K. V. Kravchyk, L. Piveteau, R. Caputo, M. He, N. P. Stadie, R. Lechner, M. V. Kovalenko*
Colloidal Bismuth Nanocrystals as a Model Anode Material for Rechargeable Mg-ion Batteries: Atomistic and Mesoscale Insights
ACS Nano, **12**, 8297-8307 (2018)

R. Caputo*
Polytypism of MoS_2
Jacobs J. Inorg. Chem., **1**, 1-10 (2016)

Y. Mettan, R. Caputo*, and T. Chatterji
A theoretical and experimental study of the crystal structure of $H_2V_3O_8$
RSC Adv., **5**, 106543-106550 (2015)

R. Caputo*, A. Kupczak, W. Sikora, and A. Tekin
Ab-initio crystal structure prediction by combining symmetry analysis representations and total energy calculations. An insight into the structure of $Mg(BH_4)_2$
Phys. Chem. Chem. Phys., **15**, 1471-1480 (2013)

R. Caputo*, A. Tekin, W. Sikora, and A. Züttel
First-principles determination of the ground-state structure of $Mg(BH_4)_2$.
Chemical Physics Letters, **480**, 203-209 (2009)

R. Caputo* and A. Tekin
Lithium dihydroborate. First-principles structure prediction of $LiBH_2$
Inorg. Chem., **51**, 9757-9765 (2012)

R. Caputo* and A. Tekin*
Ab-initio crystal structure prediction. A case study: $NaBH_4$
J. Solid State Chem., **184**, 1622-1630 (2011)

CSP

A. Tekin, R. Caputo*, and A. Züttel
First-principles determination of the ground-state structure of $LiBH_4$
Phys. Rev. Lett., **104**, 215501-215504 (2010)

Li- and Na- ion batteries

R. Caputo*
An insight into sodiation of antimony from first-principles crystal structure prediction.
Journal of Electronic Materials, **45**, 999-1010 (2016)

R. Caputo*
Exploring the structure-composition phase space of lithium borocarbide, Li_xBC for $x \leq 1$
RSC Adv., **3**, 10230-10241 (2013)

G. Zeng, R. Caputo*, D. Carriazo, L. Luo, and M. Niederberger*
Tailoring two polymorphs of $LiFePO_4$ by efficient microwave-assisted synthesis: A combined experimental and theoretical study
Chem. Mater., **25**, 3399-3407 (2013)

Optoelectronics

L. Protesescu, S. Yakunin, M. I. Bodnarchuk, F. Krieg, R. Caputo, C. Holman Hendon, R. X. Yang, A. Walsh, and M. V. Kovalenko*
Nanocrystals of cesium lead halide perovskites ($CsPbX_3$; X = Cl; Br; and I): Novel optoelectronic materials showing bright emission with wide color gamut
Nano Letters, **15**, 3692-3696 (2015)

Structure-composition-properties: Hydrogen storage

S. Garroni*, C. Milanese, D. Pottmaier, G. Mulas, P. Nolis*, A. Girella, R. Caputo, D. Olid, F. Teixidor, M. Baricco, A. Marini, S. Surinach, and M.D. Baro'
Experimental evidence of $Na_2[B_{12}H_{12}]$ and Na formation in the desorption pathway of the $2NaBH_4 + MgH_2$ system
J. Phys. Chem. C, **115**, 16664-16671 (2011)

A.J. Churchard*, E. Banach, A. Borgschulte, R. Caputo and al.
A multifaceted approach to the hydrogen storage problems
Phys. Chem. Chem. Phys., **13**, 16955-16972, 2011

R. Caputo* and A. Züttel
First-principles study of the paths of the decomposition reaction of $LiBH_4$
Mol. Phys., **108**, 1263-1276 (2010)

R. Caputo*, F. Guzzetta, and Angerhofer
Room-temperature synthesis of nickel borides via decomposition of $NaBH_4$ promoted by nickel bromide
Inorg. Chem., **49**, 8756-8762 (2010)

R. Caputo*, S. Garroni, D. Olid, F. Teixidor, S. Surinach, and M.D. Baro'
Can $Na_2[B_{12}H_{12}]$ be a decomposition product of $NaBH_4$?
Phys. Chem. Chem. Phys., **12**, 15093-15100 (2010)

P. Martelli*, R. Caputo*, A. Remhof, Ph. Mauron, A. Borgschulte, and A. Züttel
Stability and decomposition of $NaBH_4$
J. Phys. Chem. C, **114**, 7173-7177 (2010)

Hydrogen storage

R. Caputo* and A. Züttel
First-principles study of α-boron: Can the B_{12} cage host heteroatoms?
Mol. Phys., **107**, 1831-1842 (2009)

M. Matsuo, A. Remhof, P. Martelli, R. Caputo, M. Ernst, Y. Miura, T. Sato, H. Oguchi, H. Maekawa, H. Takamura, A. Borgschulte, A. Züttel, S-ichi Orimo*
Complex hydrides with (BH_4) and (NH_2) anions as new lithium fast-ion conductors
J. Amer. Chem. Soc., **131**, 16389-16391 (2009)

R. Caputo and A. Alavi*
Where do the H atoms reside in PdH_x systems?
Mol. Phys., **101**, 1781-1787 (2003)

D. Gozzi*, R. Caputo, P.L. Cignini, M. Tomellini, G. Gigli, G. Balducci, E. Cisbani, S. Frullani, F. Garibaldi, M. Jodice, G.M. Urciuoli
Calorimetric and nuclear byproducts measurements in electrochemical confinement of deuterium in palladium
J. Electroanal. Chem., **380**, 91-107, (1995)

D. Gozzi*, R. Caputo, P.L. Cignini, M. Tomellini, G. Gigli, G. Balducci, E. Cisbani, S. Frullani, F. Garibaldi, M. Jodice, G.M. Urciuoli
Quantitative measurements of helium-4 in the gas phase of Pd + D_2O electrolysis
J. Electroanal. Chem., **380**, 109-116, (1995)

Nanoparticles

M. He, L. Protesescu, R. Caputo, F. Krumeich, and M.V. Kovalenko*
A general synthesis strategy for monodisperse metallic and metalloid nanoparticles (In, Ga, Bi, Sb, Zn, Cu, Sn and their alloys) via in-situ formed metal-long-chain-amides
Chem. Mater., **27**, 635-647 (2015)

M. Yarema, M. Wörle, M.D. Rossell, R. Erni, R. Caputo, L. Protesescu, K.V. Kravchyk, D.N. Dirin, K. Lienau, F. von Rohr, A. Schilling, M. Nachtegaal, and M.V. Kovalenko*
Monodisperse colloidal gallium nanoparticles: Synthesis, low temperature crystallization, surface plasmon resonance and Li-ion storage
J. Amer. Chem. Soc., **136**, 12422-12430 (2014)

M. Yarema, R. Caputo, and M.V. Kovalenko*
Precision synthesis of colloidal inorganic nanocrystals using metal and metalloids amides
Nanoscale, **5**, 8398-8410 (2013)

Surface Reactivity

S.T. Dibaba, R. Caputo, W. Xi, R. Wei, W. Ren, and L. Sun
NIR Light Degradable Antimony Nanoparticle Based Drug Delivery System for Synergistic Chemo-Photothermal Therapy
Nanoscale (submitted)

M. Furlotti, R. Caputo, F. Krumeich, and R. Nesper*
Seamless rim-functionalization of h-BN with silica - experiment and theoretical modeling
Chem. Eur. J., **21**, 7662-7667 (2015)

Surface Reactivity

R. Caputo, B.P. Prasher, V. Stämmler, P.S. Bagus*, and Ch. Wöll
Adsorption of benzene on coinage metals: A theoretical analysis using wave-function based methods.
J. Phys. Chem. A, **111**, 12778-12784 (2007)

L.M. Ghiringhelli*, R. Caputo, and L. Delle Site*
Alkane-thiol headgroup on metal (111)-surfaces: General features of the adsorption onto group 10 and 11 transition metals
J. Phys.: Condens. Matter, **19**, 176004-1760015 (2007)

L.M. Ghiringhelli, R. Caputo, and L. Delle Site*
Phenol near Ni(111), Ni(110), and Ni(221) surfaces in a vertical ring geometry: A density functional study of the oxygen surface bonding and O-H cleavage
Phys. Rev. B, **75**, 113403-113407 (2007)

Conference Presentations and Invited Contributions (35)

Talks

R. Caputo
Firs-principles crystal structure prediction of polymorphic phases
ICMAT 2019, Singapore, 23-28 June 2019

R. Caputo
Na-Sb system: First-principles materials modelling
ICQMS International Symposium on Computational Physics
ICQMS, Shanghai University, 05 June 2018

R. Caputo
First-principles materials modeling: Crystal structure and properties prediction
ICQMS, Shanghai University, 17 May 2018

R. Caputo
First-principles materials modelling
Shanghai University, 22 June 2017

R. Caputo
First-principles crystal structure and property prediction of Li-and Na containing compounds for battery applications
3rdTYC Workshop, UCL, London, 11 September 2014

R. Caputo
First-principles crystal structure and property prediction of materials for ion-based battery applications
MSE2014, University of Darmstadt, 23 September 2014

R. Caputo
First principles crystal structure prediction
University of Southampton, Department of Chemistry, 5 March 2013

Talks

R. Caputo
Smart carbon-based materials for hydrogen storage: Theoretical results
H & E Symposium 2013, Stoos, 21 January 2013
Sinergia project *HyCarBo* meeting at the University of Parma
Department of Physics, 26 March 2013

R. Caputo
First-principles structure prediction of $LiBH_x$, x = 2.
Swiss Chemical Society, Fall meeting, ETH Zurich, 13 September 2012

R. Caputo
Are crystal structures predictable? Some case studies from first-principles approach
MPIE, Department of Interface Chemistry and Surface Engineering, Düsseldorf, 27 June 2012

R. Caputo
First-principles structure and property prediction: Li_xBC
European Scientific Symposium, Accelrys Brussels, 20 June 2012

R. Caputo
Ab-initio crystal structure prediction
Swiss Society for Crystallography, University of Bern, 16 September 2011

R. Caputo
Lithium borides: structure, lattice stability and properties. A first-principles study
ILL Grenoble, Dr. Tapan Chatterji's research group, 14 October 2011

R. Caputo
Ab-initio crystal structure prediction
Swiss Society for Crystallography, University of Bern, 16 September 2011

R. Caputo
Ab-initio crystal structure and properties predictions: Some cases study
AGH, University of Science and Technology Kraków, 30 March 2011

R. Caputo
First-principles structure and property calculations: A bridge between theory and experiments
UCL, Department of Chemistry London, 26 May 2010

R. Caputo
Bridging the length scale in computational materials science: First-principles modelling materials for hydrogen storage
Universitat Autonoma de Barcelona, Department of Physics,13 October 2009

R. Caputo
The building motif of metal tetrahydroborates: Ab-initio study
Swiss-Korean workshop, Jeju, Sud-Korea, 17-18 April 2009

Talks

R. Caputo
First-principles study of metal borides: Are they intermediates or precursor compounds for hydrogen storage?
3rd Symposium Hydrogen & Energy, Braunwald, Switzerland
25-30 January 2009

R. Caputo
First principles modelling of metal borides: Are they potential candidate materials for hydrogen storage?
ETH, Institute of Inorganic Chemistry, Zürich, 6 November 2008

R. Caputo
Metal borides from first principles approach: Lithium borides
KIST, Seoul, Sud-Korea, 28-29 April 2008

R. Caputo
Alkaline metal-boron systems: First principles calculations
2nd Symposium Hydrogen & Energy, Braunwald, Switzerland, 21-25 January 2008

R. Caputo
Adsorption on metal surfaces using density functional theory
FIAS-Frankfurt, Institute for Advanced Studies, 21 December 2005

Posters

R. Caputo
First-principles crystal structure and property prediction of compounds for energy applications
CECAM Workshop, Lausanne, 8-10 June 2015

R. Caputo
First-principles structure prediction of LiBHx; x = 2
CASTEP Workshop 2013, University of Oxford (UK), 19-23 August 2013

R. Caputo
Ab-initio crystal structure prediction. Metal borohydrides
Swiss Society for Crystallography, ETH Zurich, 21 June 2012

R. Caputo
Topologically equivalent graphitic structures
CECAM Workshop, Lausanne, 23-25 April 2012

A. Kupczak, W. Sikora, R. Caputo, and A. Tekin
Ab-initio crystal structure prediction by combining symmetry analysis representations and total energy calculations. A case study $Mg(BH_4)_2$
International Symposium on Metal-Hydrogen Systems, Kyoto, 21-26 October 2012

R. Caputo
Ab-initio crystal structure prediction
ECSSC conference, University of Lund, 25-28 September 2011

Posters

W. Sikora, R. Caputo, A. Tekin, A. Kuna, and A. Kupczak
Symmetry relations and phase stability of magnesium borohydride $Mg(BH_4)_2$
IUCr Madrid, 22-30 August 2011

R. Caputo
First-principles study of hydrogen absorption in metal borides
Gordon Research Conference, Barga (IT), July 12-17 2009

P. Martelli, A. Remhof, and R. Caputo
Stability and hydrogen desorption of $NaBH_4$
Gordon Research Conference, Barga (IT), July 12-17 2009
R. Caputo
Hydrogen-induced transformations in alkali metal-boron systems: A First principles study
International Symposium on metal hydrogen systems, University of Reykjavik, June 24-28 2008

R. Caputo
Light metal complex hydrides for hydrogen storage: Theoretical modelling
Impulse-Day at PSI, Hydrogen and Fuel Cell, Villigen (CH), November 30 2007

R. Caputo
Large molecules adsorbed on metal surfaces: a comparative DFT study
Erice School, Italy, July 2005

Granted Projects (13)

Projects

High-end Foreign Expert Project 2018, China May 2018-up to date
ICQMS, Shanghai University
Seminar lecture, contributions to current projects and initiation of new projects in materials design
Research group Prof. J. Reimers and Prof. Ren Wei

BNF projects, Universität Bern, Switzerland 2017-2018
Two collaborative projects to lead and perform computational chemistry tasks:

1.Research group Prof. A. Tekin
Technical University of Istanbul, Informatics Institute, Turkey
Title: First-principles crystal structure prediction and binary phase formation

2. KAUST, InterfacialLab, Thuwal, Saudi Arabia
Research group Prof. H. Mishra
Title: First-principles simulations of non-covalent interactions between organic molecules in water
In both projects, principal author and investigator for the computational chemistry tasks
Funds: salary

Swiss Competence Center (SCCER) Heat & Electricity Storage 2013-2015
ETH, Department of Chemistry and Applied Biosciences, Zurich, Switzerland
Research group Prof. M. Kovalenko

Projects

Title: Structures and properties of compounds for Li- and Na-ion battery applications
Contributing author and investigator for the computational chemistry tasks
Funds: salary and computational resources

Swiss National Science Foundation (SNSF) Sinergia "HyCarBo" 2010-2013
ETH, Department of Chemistry and Applied Biosciences, Zurich, Switzerland
Research group Prof. R. Nesper
Title: HyCarBo, Smart carbon-based materials for hydrogen storage
Principal author and investigator for the computational chemistry tasks
Funds: 1.5 millions Swiss francs for the 3-year project and 4 partners

Swiss-Polish PhD programme project 2010-2013
ETH, Department of Chemistry and Applied Biosciences, Zurich, Switzerland
Research group Prof. R. Nesper
Polish partner Prof W. Sikora
AGH University of Science and Technology, Kraków, Poland
Title: Multiscale modelling materials for energy applications
Principal author (at EMPA) and investigator for the computational chemistry tasks
Funds: 120000 Swiss francs

F+E-Projekte, EMPA
EMPA, Division Hydrogen & Energy, Dübendorf, Switzerland 2009-2010
Research group Prof. A. Züttel
Title: Metal-Boron systems as precursor materials for energy applications
Author and principal investigator for the computational chemistry tasks
Funds: 85000 Swiss francs

Marie Curie Research fellowship 2007-2009
EMPA, Division Hydrogen & Energy, Dübendorf, Switzerland
Research group Prof. A. Züttel
Title: Hydrogen project: Theory and modelling of complex borohydrides
Experienced researcher for the computational tasks
Funds: salary

CMA-short term visit grant April 2009
University of Liverpool, Department of Chemistry and Centre of Materials Discovery, Liverpool, UK
Research group Prof. A. Cooper
Title: Porous materials for gas storage
Principal author and investigator
Funds: travel grant

Erasmus project (part of the PhD research) 2002-2003
University of Cambridge, Department of Chemistry, Cambridge, UK
Research group Prof. A. Alavi
Title: Density functional theory (DFT) calculations applied to palladium/hydrogen systems
Pseudo-potential generation in the framework of DFT approach
Principal author and investigator of the computational and theoretical chemistry tasks
Funds: travel grant

Projects

CNR, Research Grant 1995
University of Rome “La Sapienza”, Department of Chemistry, Rome, Italy
Research group Prof. D. Gozzi
Title: Electrochemical loading of hydrogen (deuterium) in metals
Principal author and investigator of the experimental tasks
Funds: salary

Studentship Lab supervision
1992-1993
University of Rome “La Sapienza”, Department of Chemistry, Rome, Italy
Research group of Prof. E. Bottari
Title: Supervisor of undergraduate laboratory of Quantitative Analytical Chemistry
Funds: salary

Collaborations (9)

Collaborations

Prof. Jeffrey Reimers and Prof. Wei Ren 2018-up to date
ICQMS, Shanghai University
Topic: First-principles modeling of compounds for energy applications

Prof. Adem Tekin 2008-up to date
Technical University of Istanbul, Informatics Institute, Istanbul, Turkey
Topic: Crystal structure prediction via simulated annealing calculations

Prof. Himanshu Mishra 2017
KAUST, InterfacialLab, Thuwal, Saudi Arabia
Topic: Surface functionalization and interaction with organic molecules

Dr. Yoann Mettan 2010-up to date
Belenos Clean Power Holding Ltd, Itingen, Switzerland
Topic: Structure and property prediction of vanadates

Dr. Tapan Chatterji 2010-up to date
ILL, Institut Laue-Langevin, Science Division, Grenoble, France
Structure and dynamical properties of vanadates

Prof. Maksym Kovalenko 2012-2015
ETH, Department of Chemistry and Applied Biosciences, Institute of Inorganic Chemistry, Zurich
Topics: Thermal decomposition of metal / metalloid amides via molecular dynamics simulations. Crystal structure and electronic properties of compounds for solar cells, Li and Na batteries

Prof. Petr Novák's group 2014
PSI, Paul Scherrer Institute, Electrochemical Energy Storage, Villigen, Switzerland
SCCER project: Sn-based electrodes in sodium ion batteries

Prof. Wieslawa Sikora 2008-2014
AGH University of Science and Technology, Kraków, Poland
Topic: Symmetry analysis and representation of crystal structures