

Prof. Dr. Stefano Leoni

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Personal Data

Stefano Leoni, 306 David Morgan Apartments, Barry Lane, CF10 1FR, Cardiff, UK

Swiss Citizen, born 12. October 1969 in Sorengo, Switzerland

Married, 2 Kids

Mother Tongue: Italian ; French, German, English: fluent

Current Positions

- **University of Cardiff, UK**
Reader in Computational/Inorganic Chemistry
- **University of Berne, CH**
Adjoint Professor in Computational/Inorganic Chemistry

Education and Work Experience

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| 1988-1993 | ETH Zürich, Switzerland Graduate thesis
Prof. Dr. R.Nesper. |
| 1993-1998 | ETH Zürich, Switzerland PhD Thesis
Prof. Dr. R. Nesper, Prof. Dr. M. Dobler |
| 1999-2000 | ETH Zürich, Switzerland Postdoc
Institute of Inorganic Chemistry. |
| 2000 | ETH Zürich, Switzerland Postdoc
Prof. Dr. M. Gross, Computer Graphic Laboratory |
| 2000-2003 | Max Planck Institute for Chemical Physics of Solids, Dresden
Postdoc - MPG Research Scholarship
Prof. Dr. Yuri Grin and Prof. Dr. Rüdiger Kniep |
| 2002, Fall | CSCS Manno, Switzerland Guest Scientist
Prof. Dr. M. Parrinello. |
| 2004-2006 | Max Planck Institute for Chemical Physics of Solids, Dresden
Advanced Research Fellow of the SNF, Swiss National Science Foundation |
| 2005-2009 | MPI CPfS & Technical University Dresden Habilitation
<i>Venia legendi</i> in Inorganic Chemistry |

Referees: Prof. Dr. Jury Grin (MPI), Prof. Dr. Gotthard Seifert (TU-Dresden),
Prof. Dr. Michael O’Keeffe (Arizona State University).
President of the Habilitation Board: Prof. Dr. Michael Ruck.

- 2006-2010 **Max Planck Institute for Chemical Physics of Solids, Dresden**
Advanced Research Fellow MPI CPFS
- 2011-2013 **Dresden University of Technology,**
Group Leader, externally funded (DFG)
DFG Heisenberg Grant Holder
- 2012 **ETHZ, Campus USI, Lugano (March-September 2012)**
Invited Senior Researcher (Parrinello Group)
- 2012-2013 **King College London**
Invited Senior Researcher (Molteni Group)

Third Party Funds

Swiss National Science Foundation SNF Advanced Researcher Grant

Deutsche Forschungsgemeinschaft DFG LE 2479/1-1

Vorhersage, Synthese und Charakterisierung von porösen Metall-Imidazolaten MOFs.

Deutsche Forschungsgemeinschaft DFG LE 2479/1-2

Vorhersage, Synthese und Charakterisierung von porösen Metall-Imidazolaten MOFs.

Deutsche Forschungsgemeinschaft DFG LE 2479/2-1

Metastabile Metallborophosphate und Metallimidazolate mit nicht-zentrosymmetrischen Kristallstrukturen.

Deutsche Forschungsgemeinschaft DFG LE 2479/3-1

Synthese metastabiler Elementmodifikationen und Verbindungen der E13 und E14 Elemente durch kontrollierte Oxidation intermetallischer Phasen und in situ Untersuchungen der Reaktionsmechanismen.

Deutsche Forschungsgemeinschaft DFG LE 2479/2-2

Metastabile Metallborophosphate und Metallimidazolate mit nicht-zentrosymmetrischen Kristallstrukturen.

Deutsche Forschungsgemeinschaft DFG LE 2479/3-2

Synthese metastabiler Elementmodifikationen und Verbindungen der E13 und E14 Elemente durch kontrollierte Oxidation intermetallischer Phasen und in situ Untersuchungen der Reaktionsmechanismen

Invited Talks (Choice)

1. MPI PKS Dresden, IMPRS, “Molecular Dynamics Simulations of Real Materials”, 15 June 2005.
2. Università di Perugia, Theoretical Chemistry Group, “Phase Transitions in the Solid State”, Perugia, 14 February 2006.

3. ETH Zürich, Campus of the University of Lugano, Parrinello group, "Mechanisms and Intermediates along Pressure-Induced Phase Transitions", 6 March 2006.
4. EPFL Lausanne, "A Full-featured Platform for the Simulation of Phase Transitions, Mechanical Properties and Transport Phenomena in Real Materials", 11. July 2006.
5. University of Manchester, "Thinking with the Eyes", 20 April 2007.
6. National Computational Center (CSCS), Manno (Switzerland), "Numerical Simulations and Visualization Approaches", 3 March 2007.
7. North Carolina State University, ERMES Unit, "Advanced Techniques for Material Simulations", 15 March 2006.
8. National Academy of Sciences, Breslau, Poland, "Approaches to Phase Transformations in the Solid State", 18 May 2007.
9. University of Wisconsin-Madison, USA, "The Metal-Insulator Transition in MgTi₂O₄ Spinel", 15 April 2008.
10. ETH Zürich, Campus of the University of Lugano, Parrinello group, "New Results in Phase Transition Simulations", 13 August 2008.
11. TU Dresden, Nanoseminar, "Interface reactivity in Solids", 11 December 2008.
12. MPI FKF Stuttgart, Maier Group, "Numerical Simulations on nanoionics", 18 December 2008.
13. Stony Brook, New York, Center for Computational Sciences, "Understanding Structural Phase Transformations in Solids by Simulations: An Overview", 19 February 2009. (A. Oganov)
14. Arizona State University, 20 february 2009, (M. O'Keeffe)
15. "Information and Structure in the Nanoworld", St. Petersburg, 1-3 July 2009, plenary lecture.
16. MIT, Boston, 2. February 2010, Research Group of Nicola Marzari.
17. NCSU, Raleigh. 4. February 2010, Department of Chemistry. Invited Faculty Interview talk.
18. Jena, Physikalisches-Astronomische Fakultät, Symposium "Innovative Methoden der computerunterstützten Materialentwicklung", 14.-15. Februar 2011, faculty interview.
19. Miami, SMEC Conference 2011, March 2011, 2 invited talks.
20. Ulm, Symposium Anorganische Chemie, 18.-19. April 2011, faculty interview.
21. Montpellier, Euromat 2011, Highlight talk on Metallorganic Framework compounds.
22. Comenius University, Bratislava, March 2012, Martonak Group.
23. Texas University at Dallas, 6. April 2012, Chemistry/Physics Department, Buongiorno-Nardelli Group.
24. California University at Davis, Chemistry Department, April 2012, Giulia Galli & Susan Kazlarian Groups.
25. EPLF Lausanne, Mai 2012, Marzari Group, Materials Design Department.
26. MPI for Polymers, Mai 2012, Kremer Group.
27. MPI for Solid State Research, June 2012, Jansen Group.
28. Cambridge (UK), Chemistry Department, November 2012, Clare Grey Group
29. Cardiff University, Faculty Talk, February 2013.
30. University of Hamburg, Faculty talk, April 2013.
31. University of Bern, May 2013.
32. SUPSI, Lugano, June 2013.

33. University of Milan, June 2013.
34. Euromat 2013, Sevilla, September 2013.
35. Oxford University, November 2013.
36. ETH Zurich, June 2014.
37. Fock Conference, Samara August 2014