

Curriculum Vitae

Name Dr. sc. ETH Donat J. ADAMS
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Date of Birth March 19th 1977
Marital Status Single
Nationality Swiss



Education and professional activities

since Dec 2016 **Senior Assistant** at University of Bern, Institute of Geological Sciences

2010 Dec-2016 Dec **Scientist** at Empa Dübendorf in the groups of nanotech@surfaces and Reliability Science and Technology Laboratory

2009 Dec-2011 Nov **Post-doc** at the Centre de Physique Théorique (CPHT) an der École Polytechnique d'Orsay (France)

2008 Jan-2009 Nov. **Postdoctoral fellow** at the Département de Physique Théorique et Appliquée CEA

2004 Mar-2007 Oct **PhD** student at the Laboratorium f. Kristallographie, ETH Zürich. Thesis "Physics of Earth's mantle-forming minerals: electronic transitions of Fe²⁺ impurities in MgO and MgSiO₃, and phase stability of CaSiO₃ perovskite at mantle pressures and temperatures."

2003 Sep MSc (**Diploma**) in Physics, Swiss Federal Institute of Technology (ETH) Zürich. Diploma topic: "Electronic structure of 2D solids with competing periodic Potentials"

2001Sep -2002 Jun affiliated study at Eötvös Lóránd University (ELTE), Budapest with specifications on Modern solid-state Physics (theory) and Methods of solid-state Physics (experiment).

1998 Sep -2003 Jun study in physics at ETH with specifications on Solid State Theory (with G. Blatter and M. Sgrist, Institute for theoretical physics, ETH Zürich)

Teaching experience

since 2011 **lecturer** at Fachhochschule Nordwestschweiz (FHNW), School of Engineering

2014-2016 **lecturer** at EPFL (Lausanne): course on "Energy Storage" with

Prof. A. Rufer

2009 **assistant lecturer** at Ecole Polytechnique (Palaiseau, F),
Introduction to the methods of density functional theory
(4h/Woche):

2005-2007 practical training on „Fundamentals of material sciences: focus on
computational Material science“ ETHZ Zürich, (7h/Woche)

Qualifications **Doctor of Sciences** (Dr. sc. ETH Zürich, 2007)

Diploma in Physics at ETH Zürich (2003), (corresponding to a
Masters degree)

Matura, (1998) (Swiss equivalent of A-levels)

Instructor for Snowboarding and Hiking at Swiss Federal Office of
Sports (Jugend & Sport)

Languages mother-tongue German and Hungarian, good French and English

Research interests

- Life-time and safety of Li-ion batteries
- Magnetism and conductance in Nano-sized structures
- Strong correlation effects in materials
- High-pressure, high temperature prediction of phase transitions in materials
- Electronic states in aperiodic structures

Publications

Adams, D. J. and Passerone, D. (2016) Insight into structural phase transitions from
the decoupled anharmonic mode approximation, *J. Phys. Cond. Matt*, **28**, 305401

Adams, D. J. (2016) Quantum mechanical theory diffusion in solids. An application to
H in silicon and Li in LiFePO₄, *Solid State Ionics* **290**, p 116–120

Adams, D. J. et. al (2014) Identifying Photoreaction Products in Cinnamate-Based
Photoalignment Materials, *J. Phys. Chem. C*, DOI: 10.1021/jp504765f

Adams, D. J. (2014) Battery Research Platform, *hitech* **3**

Adams, D. J. et al (2012). Stable ferromagnetism and doping induced half-metallicity
in asymmetric graphene nanoribbons, *Phys. Rev. B* **85**, 245405

Adams, D. J. and Amadon, B. (2009). Study of the volume and spin collapse in
orthoferrite LuFeO₃ using LDA + U, *Phys. Rev. B* **79**, 115114.

Adams D.J., Oganov A.R. (2006). *Ab initio* molecular dynamics study of CaSiO₃
perovskite at *P-T* conditions of Earth's lower mantle. *Phys. Rev. B* **74**, art. 184106

Adams D.J., W. M. Temmerman und Z. Szotek (2009) First-principles study of the
effect of Fe impurities in MgO at geophysically relevant pressures, arXiv:0904.2901
(April 2009)

Adams D.J. und Oganov A.R. (2006). *Ab initio* molecular dynamics study of CaSiO₃
perovskite at *P-T* conditions of Earth's lower mantle. *Phys. Rev. B* **74**, 184106

Adams D.J. und Oganov A.R. Theory of minerals at extreme conditions: predictability of structures and properties in EMU Notes in Mineralogy vol.7 ("High-Pressure Behavior of Minerals", Editor R. Miletich), p. 441-457.

Presentation and Posters

"Energy Storage on an industrial level", VBSA Olten, December 2015

"Development of computational tools for molecular modelling and X-ray spectroscopy", CCMX Annual Meeting, 25.04.2012

"Characterization of conformational changes in small molecules and polymers by means of ab initio MD and X-ray absorption spectroscopy", presentation at the CECAM Workshop on X-ray Spectroscopy : Recent Advances in Modelling and New Challenges, ETH Zürich, Juli 2011

"Molecular Dynamics Simulations of cubic CaSiO₃ at lower mantle conditions" presentation at the Joint 20th AIRAPT – 43rd EHPRG International Conference on High pressure Science and Technology, Karlsruhe, June 27th – July 1st, 2005

"Theory of minerals at extreme conditions." Presentation at the Summer School of the European Mineralogical Union on "Mineral behavior at extreme conditions", Heidelberg, June 19th to 28th, 2005

"Volume and spin collapse in orthoferrite LuFeO₃ using LDA+U" at Computational Magnetism and Spintronics, International Workshop, Dresden, November 3rd - 07th, 2008

"Molecular Dynamics Simulations of cubic CaSiO₃ at lower mantle conditions" at the 20th Congress of the International Union of Crystallography, Florence, August 23rd – 31st, 2005

Further training

"Des oxydes supraconducteurs aux atomes froids: la matière à fortes corrélations quantiques " and "Correlated electrons" lecture by Prof. A. Georges, Collège de France und École polytechnique.

Fortran 95 (course 1 and 2) at Institut du développement et des ressources en informatique Scientifique (IDRIS/CNRS), Orsay, France

School on "Electronic Structure Calculations and Correlated Materials" École Predoctorale, Les Houches, France, August 27th - September 8th, 2006, Organizers: Silke Biermann, Bernard Amadon.

SIC-LSDA training with the Band Theory Group at Daresbury Laboratory, Warrington (GB). Supervisors: Prof. Walter Temmerman, Dr. D. Szotek, April 24th– 20th May 2006

CECAM/Psi-k workshop "First-Principles Simulations: Perspectives and Challenges in Mineral Sciences", Lyon, 27th September - 1st October 2004

Summer School/Conference: "Let's face Chaos through nonlinear Dynamics" Maribor (Slovenia), July 2002

Solid-State practical training at ELTE (Budapest) with Dr. Vincze Imre, September-December 2001

Prices and awards

Hubert Schleichert price, 2007