

Ing. Dominik Legut, Ph.D.

Personal data

Born: 15 December 1976 in Opava, Czech Republic
Permanent address: Jurečkova 24, CZ-746 01 Opava, Czech Republic
Nationality: Czech Republic
Married, two children

Present affiliation

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Education and professional carrier

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| <i>1995–2000</i> | student at the Brno University of Technology, Faculty of Chemistry |
| <i>1999–2000</i> | Research Assistant at the Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno |
| <i>2000–2004</i> | PhD student affiliated with the Brno University of Technology, Faculty of Chemistry, and with the Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno. PhD degree in Materials Science and Engineering. PhD Thesis: Electronic structure, displacive phase transformations and phase stability of solids. |
| <i>2005–2006</i> | Junior Research Scientist at the Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic |
| <i>2007–2009</i> | Post-doc position at Department of Physics and Materials Science, Uppsala University |
| <i>2009</i> | (3 months) Post-doc position at the Lund University |
| <i>2009–2012</i> | Post-doc position at the Material Center Leoben, Austria |
| <i>2012–present</i> | Research at the Nanotechnology Centre & IT4Innovations |

Professional experience

Field of research, specialization: theory of condensed matter, computational materials science, first-principles calculations of electronic structure of solids, displacive phase transformations in metallic materials, relativistic effects - spin-orbit interaction, elastic constants and lattice dynamics, thermal expansion, magnetism in intermetallic compounds, exchange-interactions in magnetic solids, magneto-optical effects, circularly and linearly polarized X-ray dichroism, Mössbauer spectroscopy, QMOKE

Specific topics

- effect of spin-orbit coupling along trigonal and tetragonal transformation paths in heavy elements
- magnetic behavior of Ni₃Al and Fe₃Al along displacive transformation paths
- magnetic exchange interactions in antiferromagnetic quasi-one dimensional compounds
- elastic properties of elemental metals and the influence of relativistic effects on them (spin-orbit interaction)
- magneto-optical effects in valence and x-ray regime
- X-ray magnetic circular and linear dichroism

Knowledge of languages

Mother language: Czech. Also proficient in English, partly in German, Swedish and Polish.

Experience

Full potential plane wave codes WIEN2k; pseudopotential codes VASP and Abinit; GNU/Linux Debian, grace, gnuplot, gri, Matlab/Octave/Maple, Fortran, Perl.

List of publications

Publications in reviewed journals

1. K. Carva, M. Battiato, D. Legut, and P. M. Oppeneer: Ab initio theory of electron-phonon mediated ultrafast spin relaxation of laser-excited hot electrons in transition-metal ferromagnets, *Phys. Rev. B* **87**, 184425 (2013).
2. D. Legut and U. D. Wdowik: Vibrational properties and the stability of the KCuF₃ phases, *J. Phys. Condens. Matter.* **25**, 115404 (2013).
3. R. F. Zhang, D. Legut, Z. J. Lin, Y. S. Zhao, H. K. Mao, and S. Veprek: Stability and strength of transition-metal tetraborides and triborides, *Phys. Rev. Lett.* **108**, 255502 (2012).
4. Y. Yun, D. Legut and P. M. Oppeneer: Phonon spectrum, heat capacity, and thermal expansion of UO₂ from first-principles, *J. Nucl. Mat.* **426**, 109 (2012).

5. D. Legut and J. Pavlu: Electronic structure and elasticity of Z-phases in the Cr-Nb-V-N system, *J. Phys. Condens. Matter.* **24**, 195502 (2012).
6. V. Tkáč, A. Orendáčová, M. Orendáč, K. Tibenská, A. Feher, M. Poirier, and M. W. Meisel: Experimental Study of the Thermal Transport in CsNiF₃ - An S=1 Quantum Chain, *Acta Physica Polonica A*, **121**, 1098 (2012).
7. M. Kallmayer, P. Klaer, H. Schneider, G. Jakob, H. J. Elmers, D. Legut and P. M. Oppeneer: Element-specific magnetic properties of Co₂(Mn_{1-x}Fe_x)Si films probed by x-ray magnetic circular/linear dichroism, *Phys. Rev. B* **84**, 054448 (2011).
8. F. Nolting, D. Legut, J. Ruzs, P. M. Oppeneer, G. Woltensdorf and Ch. H. Back: Anisotropy of the L_{2,3} x-ray magnetic linear dichroism of Fe films on GaAs: Experiment and *ab initio* theory, *Phys. Rev. B* **82**, 184415 (2010).
9. D. Legut and U. D. Wdowik: Ab initio study of the lattice dynamics of CsNiF₃, *J. Phys. Condens. Matter.* **22**, 435402 (2010).
10. R. F. Zhang, D. Legut, R. Niewa, A. S. Argon, and S. Veprek: Shear-induced structural transformation and plasticity in ultraincompressible ReB₂ limit its hardness, *Phys. Rev. B* **82**, 104104 (2010).
11. S. Valencia, A. Kleibert, A. Gaupp, J. Ruzs, D. Legut, J. Bansmann, W. Gudat, and P. M. Oppeneer: Quadratic X-Ray Magneto-Optical Effect upon Reflection in a Near-Normal-Incidence Configuration at the M Edges of 3d-Transition Metals, *Phys. Rev. Lett.* **104**, 187401 (2010).
12. D. Legut, M. Friák and M. Šob: Phase stability, elasticity, and theoretical strength of polonium from first principles, *Phys. Rev. B* **81**, 214118 (2010).
13. U. D. Wdowik, D. Legut and K. Ruebenbauer: Calibration of the Isomer Shift for Iodine Resonant Transitions by Ab Initio Calculations, *J. Phys. Chem. A* **114**, 7146 (2010).
14. P. Souvatzis, D. Legut, O. Eriksson and M. I. Katsnelson: Ab initio study of interacting lattice vibrations and stabilization of the β phase in Ni-Ti shape-memory alloy, *Phys. Rev. B* **81**, 092201 (2010).
15. K. Carva, D. Legut and P.M. Oppeneer: Influence of laser-excited electron distributions on the X-ray magnetic circular dichroism spectra: Implications for femtosecond demagnetization in Ni, *EPL* **86**, 57002 (2009).
16. U. D. Wdowik and D. Legut: Ab initio lattice dynamics of MnO, *J. Phys. Cond. Mat.* **21**, 275402 (2009).
17. M. Šob, D. Legut, and M. Friák: Reply to a comment, *Phys. Rev. Lett.* **102**, 079702 (2009).
18. D. Legut, M. Friák and M. Šob: Most pressurized elements aren't simple cubic, *Phys. Today* **61**, 10 (2008).
19. D. Legut: Some elements go cubic under pressure - Reply, *Phys. Today* **60**, 17 (2007).
20. M. Zelený, D. Legut, M. Šob: Ab initio study of Co and Ni under uniaxial and biaxial loading and in epitaxial overlayers, *Phys. Rev. B* **77**, 224105 (2008).

21. U.D. Wdowik and D. Legut: CoO under pressure from first principles, *J. Phys. Chem. Solids* **69**, 1698-1703 (2008).
22. D. Legut and J. Ruzs: Magnetic exchange interactions and estimation of T_N in CsNiF₃ from first principles, *Acta Physica Polonica A* **13**, 503-506 (2008).
23. D. Legut and M. Šob: Ideal tensile strength of Ni₃Al and Fe₃Al with D0₃ structure. *Mat. Sci. Forum* **567** 77-80 (2008).
24. D. Legut, M. Friák and M. Šob: Why is polonium simple cubic and so highly anisotropic?, *Phys. Rev. Lett.* **99**, 016402 (2007).
25. D. Legut and M. Šob: The loss of magnetism in tetragonally deformed Ni₃Al, *Acta Physica Slovaca* **56**, 149-152 (2006).
26. M. Zelený, D. Legut, M. Šob and J. Fiala: Ab initio study nickel along the tetragonal and trigonal deformation path, *Chem. listy* **99**, 496-498 (2005).
27. M. Šob, M. Friák, D. Legut, J. Fiala, V. Vitek: The role of ab initio electronic structure calculations in studies of the strength of materials, *Mat. Sci. Eng. A* **387**, 148-157 (2004).
28. M. Šob, D. Legut, M. Friák, J. Fiala: Magnetism of Ni₃Al and Fe₃Al under extreme pressure and shape deformation - an ab initio study, *J. Magnetism Magn. Mat.* **272**, e205-e206 (2004).

Publications in other journals

- M. Šob, M. Friák, D. Legut, V. Vitek: Strength, magnetism and stability of metals and intermetallics at extreme loading conditions (Highlight of the Month), *Psi-k Newsletter: Ab initio (from electronic structure) calculation of complex processes in materials*, No. 58 (August 2003), pp. 130–154.

Publications in monographs

- M. Šob, M. Friák, D. Legut, V. Vitek: Theoretical Strength, Magnetism and Stability of Metals and Intermetallics, *Complex Inorganic Solids - Structural, Stability, and Magnetic Properties of Alloys*, edited by P.E.A. Turchi, A. Gonis, K. Rajan and A. Meike, Springer-Verlag, Berlin-Heidelberg-New York 2005, pp. 307-326.

Highlights in brief

- Physics News Update, AIP 828 #2, June 13, 2007, <http://www.aip.org/pnu/2007/split/828-2.html> (highlighted also in *Physic Review Focus News Updates*)
- Material Research Society Bulletin vol. 32, p. 686 (2007)

Invited talks at international institutes

- UPJS Košice, Slovakia (2007)
- TU München, Garching, Germany (2008)

- UP, Krakow, Poland (2009)
- Uppsala University, Uppsala, Sweden (2009)
- IFW Dresden, Germany (2010)
- University of Regensburg, Regensburg, Germany (2013)
- GANOC, Versaille, France (2014)

Teaching experiences

- subject and laboratory: Physical chemistry at Faculty of Chemistry, Brno University of Technology (2003)
- subject and excercises: Metallic materials - Electronic structure of solids and first-principles calculations (project with LMTO code) at Faculty of Chemistry, Brno University of Technology (2004)
- talks at Students's day, Doctoral conferences VSB-TUO (2012)
- Experimental methods and nanotechnology tools II - physical methods VSB-TUO (2013)
- Modelling of the electronic structure of condensed matter (2014)

Supervisions and co-supervision

- Bachelor thesis (co-supervision): Pavlína Hemzalová - Ab initio study of electron and crystal structures of tellurium (2006)
- Master thesis (co-supervision): Monika Všianská - Electronic structure of alloys of indium and tin (2006)
- Post-Doc Mgr. Rudolf Sýkora, Ph.D. (supervision): Magnetic exchange interactions in one- and two-dimensional magnetic systems (2013)
- Post-Doc Dr. K. Lebecki (supervision): Raman and IR spectroopies induced by lattice vibrations (phonons) (2014)

Grants

- key investigatore in czech national grant (GACR, No.13-30397S): New materials for magneto-optical applications (2013-2016)
- bilateral grant with Univ. Muenster, Germany (7AMB13DE004) 2013-2014
- bilateral grant with UP Krakow, Poland (MEB051015) 2010-2011
- key person in czech national grants (GACR): Thermodynamics of intermetallic phases based on theoretical and experimental investigations (GA106/07/1078) 2007-2009, (GAP108/10/1908) 2010-2012, Theory of spin-dependent transport in magnetic solids and nanostructures (GAP204/11/1228) 2011
- 2× FRVŠ grants during Ph.D. studies (2001, 2002)