

Ing. Dominik Legut, Ph.D.

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Born: 15 December 1976 in Opava, Czech Republic
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Present affiliation

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Scientific output

- H-index **17** (April 2019)
- No. of **impacted** publications **91**, WOS
- No. of WOS citation with(without) self-citations **956(830)**
- No. of book chapters **3**

5 selected publications:

- *Theoretical Investigation of 2D Layered Materials as Protective Films for Lithium and Sodium Metal Anodes*, Adv. Ene. Mat. (2017), IF: **16.721**
- *Bright circularly polarized soft X-ray high harmonics for X-ray magnetic circular dichroism*, PNAS (2016), IF: **9.661**, cited: **48**
- *Interplay between effect of Mo and chemical disorder on the stability of beta/beta(o)-TiAl phase*, Intermetallics (2015), IF:**3.140**, cited: **11**
- *Stability and Strength of Transition-Metal Tetraborides and Triborides*, Phys. Rev. Lett. (2012), IF: **8.462**, cited: **79**
- *Why is polonium simple cubic and so highly anisotropic?*, Phys. Rev. Lett. (2007), IF: **8.462**, cited: **32**

Reviewer duties (2013-2017)

- Phys. Rev. Letters 5×, Phys. Rev. B. 5×, J. Appl. Phys. 2×, J. All. Comp. 2×, Phys. stat. sol. 5×, Mat. Chem, JACS, Phil. Mag., Surf. Coat. Comp. Mat. Des., J. Am. Cer. Soc., Mat. Des., JMMM, and etc.
- for conferences like CSMAG 2016
- for Ministry of Education (INTER-EXCELLENCE), Inter-Action USA (2017), Mobility CZ-France (2017)
- Ph.D. thesis B. Hanulíková: *Electronic properties of polysilylenes studied in silico on oligomers in various conformations*, Univ. T. Bata (2016)
- review for PRACE DECI 14th proposal 14DECI0030 *In-Silico Design of Transitional Metal Dichalcogenide Lubricants*, (2017)

Membership of societies and panels

- chairman of condensed matter physics panel of the Czech Science Foundation (2019-2021)
- vice-chairman of condensed matter physics panel of the Czech Science Foundation (2017-2019)
- guest editor of *Photonics and Nanostructures* (2017)
- member of American Physical Society (2001-2004)
- member of Czech Physical Society (2012...present)
- alumni member of Charles University (2016...present)
- member of the Newsletter editorial board of the COST Action MP 1306, *Modern Tools for Spectroscopy on Advanced Materials*, euspec.eu (2014..2018)

Invited talks at conferences and international institutes (invited by)

- UPJŠ Košice (prof. M. Orendáč), Slovakia (2007)
- TU München, (prof. S. Veprek), TU Garching, Germany (2008)
- Pedagog. Univ. (as. prof. U. D. Wdowik), Cracow, Poland (2009)
- Uppsala Univ. (prof. P. M. Oppeneer), Uppsala Sweden (2009)
- Leibnitz Inst. IFW (prof. M. Richter), Dresden Germany (2010)
- Inst. Tech. (prof. K. Watanabe), Fukuoka, Japan (2012)
- Univ. Regensburg, (prof. J. Fabian), Regensburg, Germany (2013)
- GANOC (Dr. D. Hrabovský), Versailles, France (2014)
- Univ. Hawaii, ISBB 2014 conference, Honolulu, Hawaii, USA (2014)

- Ene. Mat. Nanotech. conference (EMN 2015), Beijing, China (2015)
- Inst. Nucl. Phys. Pol. Acad. Sci., (prof. K. Parlinski), Cracow, Poland (2016)
- European Advanced Energy Materials and Technology Congress (AEMC 2018), Stockholm (2018)

Selected national and international grants, CPU proposals

Accepted:

- 20 approved CPU time projects as principal investigator (PI) at IT4Innovations (2012-2019)
- principal investigator of the PRACE DECI 10th call *EXC-XMCD*, 2 mil. corehours on TIER-1 system (2013)
- principal investigator of Czech Science Foundation grant No.17-27790S, *Novel nuclear fuel materials for IVth generation reactors* (2017-2019)
- principal investigator of multilateral (CZ-AT-SK) grant of Min. of Educ. of Czech Republic No. 8X17046, *Complex study of effects in low-dimensional quantum spin systems* (2017-2018)
- key investigator in Czech Science Foundation (GACR, No.15-08971S): *Novel nonlinear and magneto-optical phenomena in periodic structures*, (2015-2017)
- investigator in Czech Science Foundation (GACR, No.14-23274S): *Unconventional preparation of nanostructured metal oxides using overpressurized and supercritical liquids*, (2014-2015)
- investigator of the Students grants at VSB Tech. Univ. of Ostrava SP2015/71 (A. Titov, B. Kacerovská, L. Sojka, 2015), SP2016/182 (Z. Grossmanová, L. Sojka, B. Kacerovská, P. Ciompa, T. Kohut, L. Horáčková)
- key investigator in Czech Science Foundation (GACR, No.13-30397S): *New materials for magneto-optical applications*, (2013-2016)
- principal investigator of the bilateral grant with Univ. Muenster, Germany, No.7AMB13DE004 (2013-2014)
- principal investigator of the bilateral grant with Pedag. Univ. Cracow, Poland No. MEB051015 (2010-2011)
- 2× FRVŠ grants during Ph.D. studies (2001, 2002)

Submitted (role in the project):

- H2020 project (2016,2019), for more info see below (co-ordinator)
- bilateral GACR CZ-Austria 2016 (principal investigator)
- bilater Mobility projects (principal investigator): CZ-Germany (2016,2012), CZ-Austria (2016), CZ-China (2016)

- 2 GACR projects 2015 (principal investigator, key investigator)
- Visegrad fund 2014 (principal investigator)

High-Performance Computing (HPC) skills

- HPC consultant at IT4Innovations center (2015)
- PI and his collaborators consume ca. 30 millions of core-hours per year (2015-2017)
- close collaborations with HPC centers in Sweden UPPMAX-Univ. Uppsala (B. Sanyal), NSC-Univ. Linköping (P. Larsson), EPCC-Univ. Edinburgh (G. Ackland) UK, PSNC Poznań (S. Petruczynik)
- maintenance and implementation of the schedulers, load-balance systems (dqs, torque), rockscluster OS (during Ph.D. studies), administrator of two clusters at Institute of Physics of Materials, Acad. Sci. Brno (2001-2006)
- code maintainer, scaling tests on Salomon and Anselm clusters: electronic structure quantum-mechanical codes (VASP, WIEN2k, ELK, Quantum espresso, Abinit, Bethe-Salpeter code), structure prediction codes (Calypso), lattice dynamics codes (Phonopy, Phono3py, Alamode, DynaPhoPy, SCAILD)
- development of the X-ray-absorption code

Management skills

- establishing and leadership of a scientific team for the IT4Innovations National Supercomputing Center - path to exascale project research program 2 “Material’s design based on electronic structure calculations”, team consist of Dr. S. Arapan, Dr. H. Čenčariková, Dr. P. Baláž, Dr. J. Chovan, and Asoc. prof. U. D. Wdowik (September 2017)
- establishing a consortium within H2020 project No. 755532, “Novel and Advanced Nuclear Fuel Materials for generation IV Reactors - from *ab initio* to experiments” (NAFMIV) within the call NFRP-2016-2017, topic NFRP-5 consisting of 4 experimental (Helmholtz Centrum Dresden-Rosendorf (Germany), Charles University (Czech Republic), Univ. Rennes (France) and European Synchrotron Radiation Facility, Grenoble (France)) and 4 theoretical (IT4Innovations national Supercomputing center, VSB - Tech. Univ. of Ostrava (co-ordinator), Pedagog. University, Cracow (Poland), Uppsala Univ., Uppsala (Sweden), Inst. of Nucl. Sci. Pol. Acad. Sci., Cracow (Poland)) teams, total budget of 2.4mil. EUR.
- establishing a consortium for Visegrad foundation (Comenius Univ. in Bratislava, Slovakia, Pedagog. Univ. Cracow, Poland, and IT4Innovations, VSB - Tech. Univ. of Ostrava)
- principal organiser of the two days conference *Novel approaches in condensed matter physics* on May 13-14th 2015 at IT4Innovations Center within the project “New Creative Teams in Priorities of Scientific Research”, reg. no. CZ.1.07/2.3.00/30.0055.
- number of invited world-class experts that give a talk at VSB - Tech. Univ. of Ostrava, prof. P. M. Oppeneer, Uppsala Univ., Uppsala, Sweden (2012), Dr. R. Laskowski, Univ. Vienna, Vienna, Austria (2013), prof. S. Veprek, Tech. Univ. Garching, Germany (2015), Dr. J. Ruzs Uppsala Univ., Uppsala, Sweden (2017)

Supervisions and co-supervisions

- Bachelor thesis (co-supervision): Pavlína Hemzalová - Ab initio study of electron and crystal structures of tellurium FCH VUT (2006)
- Master thesis (co-supervision): Monika Všianská - Electronic structure of alloys of indium and tin, FCH VUT (2006)
- Post-Doc Mgr. Rudolf Šýkora, Ph.D. (mentor): Magnetic exchange interactions in one- and two-dimensional magnetic systems, VSB Tech. Univ. of Ostrava (2013-2015)
- Post-Doc Dr. K. Lebecki (mentor): Raman and IR spectroscopies induced by lattice vibrations, VSB Tech. Univ. of Ostrava (2014-2015)
- Bachelor thesis (supervisor): Lukáš Sojka - Electronic structure, phase stability and optical properties of Ce-doped TiO₂ phases, VSB Tech. Univ. of Ostrava (2015)
- Bachelor thesis (supervisor): Barbora Kacerovská - Electronic structure, thermal expansion and thermodynamics of U-Pu-Th carbides, VSB TUO (2015)
- Bachelor thesis (supervisor - underway): Thermal expansion of Cr- and Fe-based Zeta phases (Petr Dvoracek - VSB Tech. Univ. of Ostrava)
- Bachelor thesis (supervisor - underway): Lattice dynamics of the actinide carbides from first principles (Lukas Kyvala - VSB Tech. Univ. of Ostrava)

Teaching experiences

- Lectures and laboratory: Physical chemistry at Faculty of Chemistry, Brno University of Technology (2003).
- Lectures and exercises: Metallic materials - Electronic structure of solids and first-principles calculations (project with LMTO code) at Faculty of Chemistry, Brno University of Technology (2004).
- Experimental methods and nanotechnology tools II - physical methods VSB Tech. Univ. of Ostrava (2013-2015).
- Modelling of the electronic structure of condensed matter VSB Tech. Univ. of Ostrava (since 2014).
- Electronic structure calculations course for the HPC-study (Ph.D. study) of the IT4Innovations Center, VSB Tech. Univ. of Ostrava, (since 2015).

Education and professional carrier

<i>1995–2000</i>	MSc. 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: <i>Electronic structure, displacive phase transformations and phase stability of solids</i> .
<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>2009-2012</i>	Post-doc position at the Material Center Leoben, Austria
<i>2012-2014</i>	Senior researcher at the Nanotechnology & IT4Innovations Centers, VSB Tech. Univ. of Ostrava, Czech Republic
<i>2015-present</i>	Senior researcher and HPC consultant at IT4Innovations Center, VSB Tech. Univ. of Ostrava, Czech Republic

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, magnetism in intermetallic compounds, exchange interactions in magnetic solids, magneto-optical effects linear and quadratic in magnetization, *e.g.* circularly and linearly polarized dichroism at hard/soft X-ray and UV-VIS energy range.

Specific topics

- ultrafast demagnetization and its detection by X-ray magnetic circular dichroism
- linear and quadratic magneto-optical effects in valence and soft/hard x-ray regime
- mechanical, dynamical, and thermodynamical properties of 3D and 2D materials
- thermal expansion of materials, lattice vibrations and its anharmonic effects
- lattice dynamics and exchange interactions of quasi-1dimensional magnetic systems
- thermodynamical stability of compounds, electro-phonon coupling
- design of superhard materials and nuclear fuels
- stability of superheavy elements and calculations of the relativistic effects (spin-orbit interaction) in solids
- Li stability, nucleation, diffusion on 2D materials, solid electrolytes, protection of metal anodes

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 impacted journals

1. T. Wang, P. Zhai, D. Legut, X. Liu, Ch. Dong, Y. Fan, Y. Gong, Q. Zhang, *S-Doped Graphene-Regional Nucleation Mechanism for Dendrite-Free Lithium Metal Anodes*, Adv. Ene. Mater. (accepted 2019).
2. T. Wang, J. Qu, D. Legut, Qin, L. Jian, Z. Xifei, Q. Zhang, *Unique Double-Interstitialcy Mechanism and Interfacial Storage Mechanism in the Graphene/Metal-Oxide as Anode for Sodium-Ion Batteries*, Nano Lett. (accepted 2019).
3. F. Yanchen, T. Wang, D. Legut, and Q. Zhang, *Theoretical Investigation of Lithium Ions' Nucleation Performance on Metal-doped Cu Surfaces*, J. Ene. Chem. (accepted 2019).
4. Z.H. Fu, S.H. Zhang, S. Chen, E. Zurek, D. Legut, T.C. German, T. Lookman, and R.F. Zhang, *Anchoring Effect of Distorted Octahedra on the Stability and Strength of Platinum Metal Pernitrides*, Phys. Rev. Mater. **3**, 013603 (2019).
5. X. F. Kong, I. J. Beyerlein, Z. R. Liu, B. N. Yao, D. Legut, T. C. Germann, and R. F. Zhang, *Stronger and more failure-resistant with three-dimensional serrated bimetal interfaces*, Acta Mater. **166**, 231 (2019).
6. Y.Y. Xiao, X.F. Kong, B.N. Yao, D. Legut, T.C. Germann, R.F. Zhang, *Atomistic insight into the dislocation nucleation at crystalline/crystalline and crystalline/amorphous interfaces without full symmetry*, Acta Mater. **162**, 255 (2019).
7. J. Zhu, P. Li, X. Chen, D. Legut, Y. Fan, R. Zhang, Y. Lu, X. Cheng, and Q. Zhang, *Rational design of graphitic-inorganic Bi-layer artificial SEI for stable lithium metal anode*, Ene. Stor. Mater. **16**, 426 (2019).
8. Y. Fan, X. Chen, D. Legut, Q. Zhang, *Modeling and theoretical design of next-generation lithium metal batteries*, Ene. Stor. Mater. **16**, 169 (2019).
9. D. Legut, R. Sýkora, U. D. Wdowik, and A. Orendáčová, *Mechanical properties of the quasi-one-dimensional antiferromagnet $\text{Cu(en)(H}_2\text{O)}_2\text{SO}_4$* , J. of Nanosci. and Nanotech., **19** 3016 (2019).
10. L. Havela, M. Paukov, M. Dopita, L. Horak, D. Drozdenko, M. Divis, I. Turek, D. Legut, L. Kývala, T. Gouder, A. Seibert, F. Huber, *Crystal Structure and Magnetic Properties of Uranium Hydride UH_2 Stabilized as a Thin Film*, Inorg. Chem. **57**, 14727 (2018).

11. S.H. Zhang, X. Zheng, Q.Q. Jin, S.J. Zheng, D. Legut, X.H. Yu, H.Y. Gou, Z.H. Fu, Y.Q. Guo, B.M. Yan, C. Peng, C.Q. Jin, T.C. Germann, and R.F. Zhang, *Unprecedented plastic flow channel in γ -B₂₈ through ultrasoft bonds: A challenge to superhardness*, Phys. Rev. Mater. **2**, 123602 (2018).
12. S. Chen, Z.H. Fu, H. Zhang, D. Legut, T. C. Germann, Q. F. Zhang, S. Y. Du, J. S. Francisco, R. F. Zhang, *Surface Electrochemical Stability and Strain-Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides* Adv. Func. Mater. **28**, 1804867 (2018).
13. Z.H. Fu, S.H. Zhang, D. Legut, T.C. Germann, C. Si, S.Y. Du, J.S. Francisco, and R. Zhang, *Synergetic stabilization and strengthening strategy for two-dimensional ordered hybrid transition metal carbides*, Phys. Chem. Chem. Phys. **20**, 29684 (2018).
14. Z.H. Fu, D. Legut, T. C. Germann, C. Si, Yu. Du, J. S. Francisco, and R. F. Zhang, *Phonon-mediated stabilization and softening of 2D transition metal carbides: case studies of Ti₂CO₂ and Mo₂CO₂*, Phys. Chem. Chem. Phys. **20**, 14608 (2018).
15. S. Zhang, D. Legut, Z. Fu, T. C. Germann, and R. Zhang, *High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength*, Carbon **137**, 156 (2018).
16. M. Retuerto, S. Skiadopoulou, F. Borodavka, Ch. Kadlec, F. Kadlec, J. Prokleška, Z. Deng, J. A. Alonso, M. T. Fernandez-Diaz, F. O. Saouma, J. I. Jang, D. Legut, S. Kamba, and M. Greenblat, *Structural and spectroscopic properties of the new polar antiferromagnet Ni₂MnTeO₆*, Phys. Rev. B **97**, 144418 (2018).
17. Z. Fu; H. Zhang, Ch. Si, D. Legut, T. Germann, Q. Zhang, S. Du, J. Francisco, R. Zhang, *Mechanistic Quantification of Thermodynamic Stability and Mechanical Strength for Two-Dimensional Transition Metal Carbides*, J.Phys. Chem. C **122** 4710 (2018).
18. H. Čenčariková and D. Legut, *The effect of relativity on stability of Copernicium phases, their electronic structure and mechanical properties*, Physica B **536**, 576 (2018).
19. P. Li, J. Zhu, A. D. Handoko, R. Zhang, H. Wang, D. Legut, X. Wen, Z. Fu, Z. W. Seh and Q. Zhang, *High-throughput theoretical optimization of the hydrogen evolution reaction on MXenes by transition metal modification*, J. Mater. Chem. A **6**, 4271-4278 (2018).
20. D. Zusin, P. M. Tengdin, M. Gopalakrishnan, Ch. Gentry, A. Blonsky, M. Gerrity, D. Legut, J. M. Shaw, H. T. Nembach, T. J. Silva, P. M. Oppeneer, H. C. Kapteyn, and M. M. Murnane, *Direct measurement of the static and transient magneto-optical permittivity of cobalt across the entire M-edge in reflection geometry by use of polarization scanning*, Phys. Rev. B **97**, 024433 (2018).
21. X. Y. Chen, X. F. Konga, A. Misrab, D. Legut, B. N. Yao, T. C. Germann, and R. F. Zhang, *Effect of dynamic evolution of misfit dislocation pattern on dislocation nucleation and shear sliding at semi-coherent bimetal interfaces* Acta Materialia **143**, 107 (2018).
22. H. Zhang, Z. Fu, R. Zhang, Q. Zhang, H. Tian, D. Legut, T. C. Germann, Y. Guoa, S. Due, and J. S. Francisco *Designing flexible 2D transition metal carbides with strain-controllable lithium storage*, Proc. Nat. Acad. USA **114**, E11082-E11091 (2017).

23. H. Zhang, Z. H. Fu, D. Legut, T. C. Germann and R. F. Zhang, *Stacking stability and sliding mechanism in weakly bonded 2D transition metal carbides by van der Waals force*, RSC Adv. **7**, 55912-55919 (2017).
24. Mat. Mihalik, Mar. Mihalik, A. Hoser, D. M. Pajerowski, D. Kriegner, D. D. Legut, K. M. Lebecki, M. Vavra, M. Fitta, M. W. Meisel, *Magnetic structure of the mixed antiferromagnet $\text{NdMn}_{0.8}\text{Fe}_{0.2}\text{O}_3$* , Phys. Rev. B **96**, 134430 (2017).
25. S. Borroni, E. Baldini, V. M. Katukuri, A. Mann, K. Parlinski, D. Legut, C. Arrell, F. van Mourik, J. Teyssier, A. Kozłowski, P. Piekarczyk, O. V. Yazyev, A. M. Oleś, J. Lorenzana, and F. Carbone, *Coherent generation of symmetry-forbidden phonons by light-induced electron-phonon interactions in magnetite* Phys. Rev. B **96**, 104308 (2017).
26. R. F. Zhang, X. F. Kong, H. T. Wang, S. H. Zhang, D. Legut, S. H. Sheng, S. Srinivasan, K. Rajan, and T. C. Germann, *An informatics guided classification of miscible and immiscible binary alloy systems*, Sci. Rep. **7**, 9577 (2017).
27. S. H. Zhang, I. J. Beyerlein, D. Legut, Z. H. Fu, Z. Zhang, S. L. Shang, Z. K. Liu, T. C. Germann, and R. F. Zhang. *First-principles investigation of strain effects on the stacking fault energies, dislocation core structure, and Peierls stress of magnesium and its alloys*, Phys. Rev. B **95**, 224106 (2017).
28. H. Tian, Z. W. Seh, K. Yan, Z. Fu, P. Tang, Y. Lu, R. Zhang, D. Legut, Y. Cui, Q. Zhang, *Theoretical Investigation of Two-Dimensional Layered Materials as Protective Films for Lithium and Sodium Metal Anodes*, Advan. Ene. Mat. **7**, 1602528 (2017).
29. G. Rogl, D. Legut, R. Sýkora, P. Müller, H. Müller, E. Bauer, S. Puchegger, M. Zehetbauer, and P. Rogl, *Mechanical properties of non-centrosymmetric CePt_3Si and CePt_3B* , J. Phys. Cond. Matt. **29**, 185402 (2017).
30. L. Lederová, A. Orendáčová, J. Chovan, J. Strečka, T. Verkholyak, R. Tarasenko, D. Legut, R. Sýkora, E. Čížár, V. Tkáč, M. Orendáč, and A. Feher, *Realization of a spin- $\frac{1}{2}$ spatially anisotropic square lattice in a quasi-two-dimensional quantum antiferromagnet $\text{Cu(en)}(\text{H}_2\text{O})_2\text{SO}_4$* , Phys. Rev. B **95**, 054436 (2017).
31. H.-Ch. Mertins, C. Jansing, M. Gilbert, M. Krivenkov, J. Sanchez-Barriga, A. Varykhalov, O. Rader, H. Wahab, H. Timmers, A. Gaupp, M. Tesch, A. Sokolov, D. Legut and P. M. Oppeneer, *Magneto-optical reflection spectroscopy on graphene/Co in the soft x-ray range*, J. Phys. Conf. Ser. **903**, 012025 (2017).
32. E. Turgut, D. Zusin, D. Legut, K. Carva, R. Knut, J. Shaw, C. Chen, Z. Tao, H. Nembach, T. J. Silva, S. Mathias, M. Aeschlimann, P. M. Oppeneer, H. C. Kapteyn, M. M. Murnane, and P. Grychtol, *Stoner vs. Heisenberg: Ultrafast exchange reduction and magnon generation during laser-induced demagnetization*, Phys. Rev. B **94**, 220408(R) (2016).
33. J. Hamrlová, D. Legut, M. Veis, J. Pištora, and J. Hamrle, *Principal spectra describing magnetooptic permittivity tensor in cubic crystals*, J. Magn. Mag. Mat. **420**, 143 (2016).
34. U. D. Wdowik, P. Piekarczyk, D. Legut, and G. Jagło, *Effect of spin-orbit and on-site Coulomb interactions on the electronic structure and lattice dynamics of uranium monocarbide*, Phys. Rev. B **94**, 054303 (2016).

35. Z. H. Fu, Q. F. Zhang, D. Legut, C. Si, T. C. Germann, T. Lookman, S. T. Du, J. S. Francisco, R. F. Zhang, *Stabilization and strengthening effects of functional groups in two-dimensional titanium carbide*, Phys. Rev. B **94**, 104103 (2016).
36. C. Jansing, H.-Ch. Mertins, M. Gilbert, H. Wahab, H. Timmers, S.-H. Choi, A. Gaupp, M. Krivenkov, A. Varykhalov, O. Rader, D. Legut, and P. M. Oppeneer, *X-ray natural birefringence in reflection from graphene*, Phys. Rev. B **94**, 045422 (2016).
37. Z. Zhang, R. F. Zhang, D. Legut, D. Q. Li, S. H. Zhang, Z. H. Fu, and H. B. Guo, *Pinning effect of reactive elements on adhesion energy and adhesive strength of incoherent $Al_2O_3/NiAl$ interface*, Phys. Chem. Chem. Phys. **18**, 22864 (2016).
38. T. Káňa, E. Hüger, D. Legut, M. Čák, and M. Šob, *Magnetism and deformation of epitaxial Pd and Rh thin films*, Phys. Rev. B **93**, 134422 (2016).
39. Z. J. He, Z. H. Fu, D. Legut, X. H. Yu, Q. F. Zhang, V. I. Ivashchenko, S. Veprek, and R. F. Zhang, *Tuning lattice stability and mechanical strength of ultra-incompressible tungsten carbides by varying the stacking sequence*, Phys. Rev. B **93**, 184104 (2016).
40. K. Lebecki and D. Legut, *Fast vortex core switching at high temperatures*, J. Magn. Mag. Mat. **411**, 7 (2016).
41. R.F. Zhang, X.D. Wen, D. Legut, Z.H. Fu, S. Veprek, E. Zurek and H.K. Mao, *Crystal Field Splitting is Limiting the Stability and Strength of Ultra-incompressible Orthorhombic Transition Metal Tetraborides* Sci. Rep. **6**, 23088 (2016)
42. Z. Zhang, Z.H. Fu, R.F. Zhang, D. Legut, and H.B. Guo, *Anomalous mechanical strengths and shear deformation paths of Al_2O_3 polymorphs with high ionicity*, RSC Adv. **6**, 12885 (2016).
43. K. Lebecki and D. Legut, *Bloch-point velocity in square ferromagnetic nanowires - temperature-aware micromagnetic simulations*, Advanced Science Letters **22**, 622 (2016).
44. R. Sýkora K. Postava, D. Legut and R. Tarasenko, *Calculated Reflection Coefficients of a Single Planar Interface with an Optically Biaxial $Cu(en)(H_2O)_2 SO_4$ - Material Compared to Experiment*, Journal of Nanoscience and Nanotechnology, **16**, 7818 (2016).
45. T. Fan, P. Grychtol, R. Knut, C. Hernández-García, D. D. Hickstein, D. Zusin, Ch. Gentry, F. Dollar, Ch. Mancuso, C. W. Hogle, O. Kfir, D. Legut, K. Carva, J. L. Ellisa, K. Dorneya, C. Chena, O. G. Shpyrko, E. E. Fullertonh, O. Cohenc, P. M. Oppeneer, D. B. Milošević, A. Becker, A. A. Jaron-Becker, T. Popmintcheva, M. M. Murnanea, and H. C. Kapteyn, *Bright circularly polarized soft X-ray high harmonics for X-ray magnetic circular dichroism*, Proc. Nat. Acad. USA **112**, 14206 (2015).
46. R. F. Zhang, D. Legut, Z. H. Fu, S. Veprek, Q. F. Zhang, and H. K. Mao, *Mechanical strength and electronic instabilities in ultra-incompressible platinum dinitrides*, Phys. Rev. B **92**, 104107 (2015).
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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)