Curriculum Vitae of

Priv.-Doz. Mgr. David Holec, PhD

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Education and academic qualifications

2016	Habilitation in the field of "Computational Materials Science" (Priv.-Doz.), Montanuniversität Leoben, AT Thesis: *First principles modelling of alloying trends*
2005–2008	PhD in Material Science, University of Cambridge, Cambridge, UK Dissertation: *"Multi-scale modelling of III-nitrides: from dislocations to the electronic structure"*
2003–2005	Mgr. (equiv. to MSc) in Physics of Condensed Matter, Masaryk University, Brno, CZ Diploma work: *"On the precipitation in NiTi based shape memory alloys"*
1999–2004	Bc. (equiv. to BSc) in Physics, Masaryk University, Brno, CZ Bachelor's project: *"On the motion of low-angle dislocation boundaries in precipitation hardened systems"*
1999–2002	Bc. (equiv. to BSc) in Mathematics, Masaryk University, Brno, CZ Bachelor's project: *"Differential geometry of curves related to a physical practice"*

Career development

2019–	Senior Lecturer and Group leader "Materials Modelling Group", Dept. of Materials Science, Montanuniversität Leoben, Leoben, AT
09–12/2018	Guest Professor, Inst. of Materials Science and Technology TU Wien, Vienna, AT
2018–2019	Visiting scientist at RWTH Aachen, DE (5 weeks)
2017–2018	Senior Lecturer and Group leader "Materials Modelling Group", Dept. of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, AT
2015–2018	Visiting scientist at the Central South University, Chagsha, CN (8 weeks)
2015–	Guest lecturer, Inst. of Materials Science and Technology, TU Wien, Vienna, AT
2013–	Guest researcher, Inst. of Materials Science and Technology, TU Wien, Vienna, AT
2010–2017	University assistant, Dept. of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, AT
2008–2010	Postdoctoral research fellow, Dept. of Physical Metallurgy and Materials Testing, Montanuniversität, Leoben, AT
2005–2008	Marie Curie early stage researcher, University of Cambridge, Cambridge, UK
2003–2005	Research fellow, Inst. of Physics of Materials, Academy of Sciences, Brno, CZ
2001–2003	Tutor of mathematical seminars, Faculty of Informatics, Masaryk Univ., Brno, CZ

Research activities and interests

- *ab initio* calculations of structural properties (phase stability, mechanical and thermodynamic properties), electronic structure, phase transformations
- atomistic modelling (molecular dynamics, Monte Carlo) of size effects in nanostructures;
- a multimethod/multiscale approach (from quantum to classical mechanics) to material science problems (polycrystalline and hierarchical structures); *ab initio*-powered Calphad modelling
- defect engineering, e.g. stabilisation by point defects, alloying impact on stacking faults, mobility of dislocations
- hydrogen storage
- material systems: functional coatings (nitrides, oxides, borides); steels; TiAl and related intermetallic alloys; shape memory alloys; C and Au nanostructures

Dissemination of the results (Scopus, June 2023)

peer-reviewed publication:	186
h-index:	37 (excluding self-citations of all authors: 32)
citations:	4561 (excluding self-citations of all authors: 3205)
list of all publications:	cms.unileoben.ac.at/download/CV-David_Holec.pdf
invited conference presentations:	20

Selected projects

2022–2029	"Knowledge-based Design of Advanced Steels (KnowDAS)" [CDG], area leader
2021–2024	"Additive Manufacturing of Non-Weldable Nickel-Base Superalloys: Process, Microstrucutre and Mechanical Properties" [FFG Bridge], project partner
2021–2022	"Impact of hydrogen on structural and functional properties of NiTi shape memory alloys" [OeAD-WTZ], bi-lateral mobility project with CZ, Austrian co-PI
2020–2023	"Cross-Sectional Microstructure and Stress Design of Tough Diamond Coatings" [FFG Bridge], project partner
2019–2022	"Diffusion control reducing friction of nanocomposite materials" [FWF/GAČR], international joint project with CZ, Austrian co-PI
2018–2022	"Computational-assisted Process Development and Materials Design of Novel CVD Hard Coatings (NovelCVD) " [FFG Comet], key researcher
2017–2021	"Atomistic Principles of Martensitic and Ordering Transformations in Intermetallic Alloys at Finite Temperatures (MOTIF)" [FWF], PI
2017–2020	"Impact of interfaces on mechanical properties of hard coating materials" [FWF], co-PI
2017–2020	"Erosion behaviour of composite AlCr arc cathodes" [FFG Bridge], project partner

Teaching and mentoring experience

- currently supervising 4 PhD students, 5 Master and 1 Bachelor students, all working in the field of atomistic and electronic structure calculations.

	Postdoc	*PhD*	*Master*	*Bachelor*
Finished	3 (+1 co-advised)	2 (+10 co-advised)	12	8
Ongoing	0	5 (+2 co-advised)	3	0

- teaching courses on "Dislocations and Elasticity", "Atomistic Modelling", "Solid State Physics" and "Physical Metallurgy" (Montanuniversität Leoben)
- teaching courses on "Dislocations and Elasticity", "Atomistic Materials Modelling" (TU Wien)

Professional affiliations

- Deutsche Physikalische Gesellschaft (DPG)

5 most important scientific achievements

1. ASMET-Forschungspreis 2016 (Feb 2017, 300k€)
2. Theodor Körner Preis, "Understanding the response of filled carbon nanotubes to an applied external stimulus" (Apr 2011, 3k€)
3. PI and co-PI of 3 FWF projects, co-investigator of 4 FFG and 1 FWF project, principle researcher of 2 FFG-Comet projects, area leader of 1 CDL, PI and co-PI of 5 OeAD-WTZ projects
4. reviewer for Phys. Rev. B, Phys. Rev. Lett, Acta Mat., Sci. Rep., Vacuum, Comp. Mat. Sci., Surf. Coat. Technol., Thin Films, J. Phys. D: Appl. Phys, J. Appl. Phys, J. Phys: Cond. Matter, Appl. Lett., Mat. Sci. Eng., Phil. Mag. and other journals
5. session/symposium organiser at ICMCTF (International Conference on Metallurgical Coatings and Thin Films), CA, USA (2012–2014, 2018, 2020–2022); MSE Congress (Materials Science and Engineering), Darmstadt, DE (2022); Euromat, Graz, AT (2021), ECCOMAS (European Congress on Computational Methods in Applied Sciences and Engineering), Vienna (2012); Austrian-German Workshop on Computational Materials Design, Kirchdorf, AT (2012, 2015, 2018)

5 selected most relevant recent publications

1. D. Gehringer, M. Friák, and D. Holec. Models of configurationally-complex alloys made simple. *Comput. Phys. Commun.*, 286:108664, 2023. doi: 10.1016/j.cpc.2023.108664
2. N. Abdoshahi, M. Dehghani, A. V. Ruban, M. Friák, M. Šob, J. Spitaler, and D. Holec. On the energetics of the cubic-to-hexagonal transformations in TiAl+Mo alloys. *Acta Mater.*, 240: 118268, 2022. doi: 10.1016/j.actamat.2022.118268
3. M. Dehghani, A. V. Ruban, N. Abdoshahi, D. Holec, and J. Spitaler. Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. *Comput. Mater. Sci.*, 205:111163, 2022. doi: 10.1016/j.commatsci.2021.111163
4. N. Abdoshahi, M. Dehghani, L. Hatzenbichler, P. Spoerk-Erdely, A. V. Ruban, M. Musi, S. Mayer, J. Spitaler, and D. Holec. Structural stability and mechanical properties of TiAl+Mo alloys: A comprehensive ab initio study. *Acta Mater.*, 221:117427, 2021. doi: 10.1016/j.actamat.2021.117427
5. O. Schneeweiss, M. Friák, M. Dudová, D. Holec, M. Šob, D. Kriegner, V. Holý, P. Beran, E. P. George, J. Neugebauer, and A. Dlouhý. Magnetic properties of the CrMnFeCoNi high-entropy alloy. *Phys. Rev. B Condens. Matter*, 96(1):014437, 2017. doi: 10.1103/PhysRevB.96.014437

Publications

Peer-reviewed publications

1. G. Graf, M. Seyffertitz, P. Spoerk-Erdely, H. Clemens, A. Stark, L. Hatzenbichler, D. Holec, M. Burtscher, D. Kiener, X. Li, and K. Liu. On the stability of Ti(Mn,Al)2 C14 laves phase in an intermetallic Ti–42Al–5Mn alloy. *Intermetallics*, 161(107962):107962, 2023. doi: 10.1016/j.intermet.2023.107962
2. G. K. Nayak, D. Holec, and M. Zelený. Impact of d-states on transition metal impurity diffusion in TiN. *Sci. Rep.*, 13(1):8244, 2023. doi: 10.1038/s41598-023-34768-7
3. G. K. Nayak, A. Kretschmer, P. H. Mayrhofer, and D. Holec. On correlations between local chemistry, distortions and kinetics in high entropy nitrides: An ab initio study. *Acta Mater.*, 255:118951, 2023. doi: 10.1016/j.actamat.2023.118951
4. L. Hatzenbichler, S. Zeisl, H. Clemens, and D. Holec. Phase stability of TiAl-based BCC high entropy alloys. *Intermetallics*, 158:107893, 2023. doi: 10.1016/j.intermet.2023.107893
5. D. Gehringer, M. Friák, and D. Holec. Models of configurationally-complex alloys made simple. *Comput. Phys. Commun.*, 286:108664, 2023. doi: 10.1016/j.cpc.2023.108664
6. I. J. Gómez, M. V. Sulleiro, N. Pizúrová, A. Bednařík, P. Lepcio, D. Holec, J. Preisler, and L. Zajíčková. Spontaneous formation of carbon dots helps to distinguish molecular fluorophores species. *Appl. Surf. Sci.*, 610:155536, 2023. doi: 10.1016/j.apsusc.2022.155536
7. J. Li, X. Zhou, A. Breen, Z. Peng, J. Su, P. Kürnsteiner, M. J. D. Correa, M. L. Chwałek, H. Wang, D. Holec, J. Mayer, and G. Dehm. Elucidation of formation and transformation mechanisms of ca-rich laves phase in Mg-Al-Ca-Mn alloys. *J. Alloys Compd.*, 928(167177): 167177, 2022. doi: 10.1016/j.jallcom.2022.167177
8. L. Michal, R. Roy, D. Holec, I. J. Gómez, N. Pizúrová, D. Nečas, A. Dolečková, J. Medalová, P. Lepcio, and L. Zajíčková. Long-Range magnetic order in nickel Hydroxide-Functionalized graphene quantum dots. *J. Phys. Chem. Lett.*, 13(49):11536–11542, 2022. doi: 10.1021/acs.jpclett.2c02964
9. M. Musi, S. Kardos, L. Hatzenbichler, D. Holec, A. Stark, M. Allen, V. Güther, H. Clemens, and P. Spoerk-Erdely. The effect of zirconium on the ti-(42-46 at.%)al system. *Acta Mater.*, 241:118414, 2022. doi: 10.1016/j.actamat.2022.118414
10. N. Abdoshahi, M. Dehghani, A. V. Ruban, M. Friák, M. Šob, J. Spitaler, and D. Holec. On the energetics of the cubic-to-hexagonal transformations in TiAl+Mo alloys. *Acta Mater.*, 240: 118268, 2022. doi: 10.1016/j.actamat.2022.118268
11. A. Sakic, C. Hofer, R. Schnitzer, and D. Holec. Ab initio study of alloying impact on the stability of cementite in transformation-induced plasticity-assisted advanced steels. *Adv. Eng. Mater.*, page 2200532, 2022. doi: 10.1002/adem.202200532
12. J. Li, X. Zhou, A. Breen, Z. Peng, J. Su, P. Kürnsteiner, M. J. D. Correa, M. L. Chwałek, H. Wang, D. Holec, J. Mayer, and G. Dehm. Elucidation of formation and transformation mechanisms of ca-rich laves phase in Mg-Al-Ca-Mn alloys. *J. Alloys Compd.*, 928:167177, 2022. doi: 10.1016/j.jallcom.2022.167177
13. M. Meindlhumer, T. Ziegelwanger, J. Zalesak, M. Hans, L. Löfler, S. Spor, N. Jäger, A. Stark, H. Hruby, R. Daniel, D. Holec, J. M. Schneider, C. Mitterer, and J. Keckes. Precipitation-based grain boundary design alters inter- to trans-granular fracture in AlCrN thin films. *Acta Mater.*, 237:118156, 2022. doi: 10.1016/j.actamat.2022.118156

14. M. Hans, Z. Czigány, D. Neuß, J. A. Sälker, H. Rueß, J. Krause, G. K. Nayak, D. Holec, and J. M. Schneider. Probing the onset of wurtzite phase formation in (v, al) N thin films by transmission electron microscopy and atom probe tomography. *Surf. Coat. Technol.*, page 128235, 2022

15. R. Roy, D. Holec, M. Kratzer, P. Muenzer, P. Kaushik, L. Michal, G. S. Kumar, L. Zajíčková, and C. Teichert. Probing the charge transfer and electron-hole asymmetry in graphene-graphene quantum dot heterostructure. *Nanotechnology*, 33(32), 2022. doi: 10.1088/1361-6528/ac6c38

16. J. Buchinger, N. Koutná, A. Kirnbauer, D. Holec, and P. H. Mayrhofer. Heavy-element-alloying for toughness enhancement of hard nitrides on the example Ti-W-N. *Acta Mater.*, page 117897, 2022

17. Y. W. Sun, D. Holec, D. Gehringer, L. Li, O. Fenwick, D. J. Dunstan, and C. J. Humphreys. Graphene on silicon: Effects of the silicon surface orientation on the work function and carrier density of graphene. *Phys. Rev. B Condens. Matter*, 105(16):165416, 2022. doi: 10.1103/PhysRevB.105.165416

18. P. Ondračka, M. Hans, D. M. Holzapfel, D. Primetzhofer, D. Holec, and J. M. Schneider. Ab initio-guided X-ray photoelectron spectroscopy quantification of Ti vacancies in $Ti_{1-\delta}O_xN_{1-x}$ thin films. *Acta Mater.*, 230(117778):117778, 2022. doi: 10.1016/j.actamat.2022.117778

19. N. Koutná, L. Löfler, D. Holec, Z. Chen, Z. Zhang, L. Hultman, P. H. Mayrhofer, and D. G. Sangiovanni. Atomistic mechanisms underlying plasticity and crack growth in ceramics: a case study of AlN/TiN superlattices. *Acta Mater.*, page 117809, 2022. doi: 10.1016/j.actamat.2022.117809

20. J. Ženíšek, P. Ondračka, J. Čechal, P. Souček, D. Holec, and P. Vašina. W 4f electron binding energies in amorphous W-B-C systems. *Appl. Surf. Sci.*, 586:152824, 2022. doi: 10.1016/j.apsusc.2022.152824

21. F. Schmid, D. Gehringer, T. Kremmer, L. Cattini, P. J. Uggowitzer, D. Holec, and S. Pogatscher. Stabilization of Al_3Zr allotropes in dilute aluminum alloys via the addition of ternary elements. *Materialia*, 21:101321, 2022. doi: 10.1016/j.mtla.2022.101321

22. M. Dehghani, A. V. Ruban, N. Abdoshahi, D. Holec, and J. Spitaler. Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. *Comput. Mater. Sci.*, 205:111163, 2022. doi: 10.1016/j.commatsci.2021.111163

23. M. Tkadletz, N. Schalk, A. Lechner, L. Hatzenbichler, D. Holec, C. Hofer, M. Deluca, B. Sartory, A. Lyapin, J. Julin, and C. Czettl. Influence of B content on microstructure, phase composition and mechanical properties of CVD Ti(B,N) coatings. *Materialia*, 21:101323, 2022. doi: 10.1016/j.mtla.2022.101323

24. A. Kretschmer, D. Holec, K. Yalamanchili, H. Rudigier, M. Hans, J. M. Schneider, and P. H. Mayrhofer. Strain-stabilized al-containing high-entropy sublattice nitrides. *Acta Mater.*, 224:117483, 2022. doi: 10.1016/j.actamat.2021.117483

25. Y. W. Sun, D. Gehringer, D. Holec, D. G. Papageorgiou, O. Fenwick, S. M. Qureshi, C. J. Humphreys, and D. J. Dunstan. Significant interlayer coupling in bilayer graphene and double-walled carbon nanotubes: A refinement of obtaining strain in low-dimensional materials. *Phys. Rev. B Condens. Matter*, 105(2):024103, 2022. doi: 10.1103/PhysRevB.105.024103

26. N. Abdoshahi, M. Dehghani, L. Hatzenbichler, P. Spoerk-Erdely, A. V. Ruban, M. Musi, S. Mayer, J. Spitaler, and D. Holec. Structural stability and mechanical properties of TiAl+Mo alloys: A comprehensive ab initio study. *Acta Mater.*, 221:117427, 2021. doi: 10.1016/j.actamat.2021.117427

27. D. Holec, N. Abdoshahi, D. Gehringer, L. Hatzenbichler, A. Sakic, and H. Clemens. Electrons meet alloy development: a γ-TiAl-based alloys showcase. *Adv. Eng. Mater.*, 2021. doi: 10.1002/adem.202100977

28. L. Löfler, R. Hahn, P. H. Mayrhofer, M. Bartosik, and D. Holec. Mechanical properties of CrN-based superlattices: Impact of magnetism. *Acta Mater.*, 218:117095, 2021. doi: 10.1016/j.actamat.2021.117095

29. D. M. Holzapfel, Music, Denis, M. Hans, S. Wolff-Goodrich, D. Holec, D. Bogdanovski, M. Arndt, A. O. Eriksson, K. Yalamanchili, D. Primetzhofer, C. H. Liebscher, and J. M. Schneider. Enhanced thermal stability of (Ti,Al)N coatings by oxygen incorporation. *Acta Mater.*, 218:117204, 2021. doi: 10.1016/j.actamat.2021.117204

30. G. K. Nayak, M. N. Popov, and D. Holec. Pressure- and temperature-dependent diffusion from first-principles: A case study of V and ti in a TiN matrix. *Surf. Coat. Technol.*, 422:127491, 2021. doi: 10.1016/j.surfcoat.2021.127491

31. Z. Chen, Y. Zheng, L. Löfler, M. Bartosik, G. K. Nayak, O. Renk, D. Holec, P. H. Mayrhofer, and Z. Zhang. Atomic insights on intermixing of nanoscale nitride multilayer triggered by nanoindentation. *Acta Mater.*, 214:117004, 2021. doi: 10.1016/j.actamat.2021.117004

32. Z. Zhang, A. Ghasemi, N. Koutná, Z. Xu, T. Grünstäudl, K. Song, D. Holec, Y. He, P. H. Mayrhofer, and M. Bartosik. Correlating point defects with mechanical properties in nanocrystalline TiN thin films. *Mater. Des.*, 207:109844, 2021. doi: 10.1016/j.matdes.2021.109844

33. D. Holec, L. Löfler, G. A. Zickler, D. Vollath, and F. D. Fischer. Surface stress of gold nanoparticles revisited. *Int. J. Solids Struct.*, 224:111044, 2021. doi: 10.1016/j.ijsolstr.2021.111044

34. Y. W. Sun, D. Holec, D. Gehringer, O. Fenwick, D. J. Dunstan, and C. J. Humphreys. Erratum: Unexpected softness of bilayer graphene and softening of A-A stacked graphene layers [phys. rev. B 101, 125421 (2020)]. *Phys. Rev. B Condens. Matter*, 103(11):119901, 2021. doi: 10.1103/PhysRevB.103.119901

35. A. Wagner, D. Holec, P. H. Mayrhofer, and M. Bartosik. Enhanced fracture toughness in ceramic superlattice thin films: On the role of coherency stresses and misfit dislocations. *Materials and Design*, 202, 2021. doi: 10.1016/j.matdes.2021.109517

36. Z. Chen, Y. Zheng, L. Löfler, M. Bartosik, H. Sheng, C. Gammer, D. Holec, and Z. Zhang. Real-time atomic-resolution observation of coherent twin boundary migration in CrN. *Acta Mater.*, 208:116732, 2021. doi: 10.1016/j.actamat.2021.116732

37. F. F. Klimashin, L. Lobmaier, N. Koutná, D. Holec, and P. H. Mayrhofer. The MoN–TaN system: Role of vacancies in phase stability and mechanical properties. *Mater. Des.*, 202:109568, 2021. doi: 10.1016/j.matdes.2021.109568

38. N. Koutná, A. Brenner, D. Holec, and P. H. Mayrhofer. High-throughput first-principles search for ceramic superlattices with improved ductility and fracture resistance. *Acta Mater.*, 206: 116615, 2021. doi: 10.1016/j.actamat.2020.116615

39. J. Buchinger, A. Wagner, Z. Chen, Z. L. Zhang, D. Holec, P. H. Mayrhofer, and M. Bartosik. Fracture toughness trends of modulus-matched TiN/(Cr,Al)N thin film superlattices. *Acta Mater.*, 202:376–386, 2021. doi: 10.1016/j.actamat.2020.10.068

40. N. Abdoshahi, P. Spoerk-Erdely, M. Friák, S. Mayer, M. Šob, and D. Holec. Ab initio study of chemical disorder as an effective stabilizing mechanism of bcc-based TiAl+Mo. *Phys. Rev. Materials*, 4(10):103604, 2020. doi: 10.1103/PhysRevMaterials.4.103604

41. J. Buchinger, L. Löfler, J. Ast, A. Wagner, Z. Chen, J. Michler, Z. L. Zhang, P. H. Mayrhofer, D. Holec, and M. Bartosik. Fracture properties of thin film TiN at elevated temperatures. *Mater. Des.*, 194:108885, 2020. doi: 10.1016/j.matdes.2020.108885

42. F. Anğay, L. Löfler, F. Tetard, D. Eyidi, P. Djemia, D. Holec, and G. Abadias. Structure, stress, and mechanical properties of Mo-Al-N thin films deposited by dc reactive magnetron cosputtering: Role of point defects. *J. Vac. Sci. Technol. A*, 38(5):053401, 2020. doi: 10.1116/6.0000292

43. R. Hahn, N. Koutná, T. Wójcik, A. Davydok, S. Kolozsvári, C. Krywka, D. Holec, M. Bartosik, and P. H. Mayrhofer. Mechanistic study of superlattice-enabled high toughness and hardness in MoN/TaN coatings. *Communications Materials*, 1(1):62, 2020. doi: 10.1038/s43246-020-00064-4

44. Z. Zhang, Z. Chen, D. Holec, C. H. Liebscher, N. Koutná, M. Bartosik, Y. Zheng, G. Dehm, and P. H. Mayrhofer. Mapping the mechanical properties in nitride coatings at the nanometer scale. *Acta Mater.*, 2020. doi: 10.1016/j.actamat.2020.04.024

45. F. Moitzi, D. Şopu, D. Holec, D. Perera, N. Mousseau, and J. Eckert. Chemical bonding effects on the brittle-to-ductile transition in metallic glasses. *Acta Mater.*, 188:273–281, 2020. doi: 10.1016/j.actamat.2020.02.002

46. P. Ondračka, D. Nečas, M. Carette, S. Elisabeth, D. Holec, A. Granier, A. Goullet, L. Zajíčková, and M. Richard-Plouet. Unravelling local environments in mixed TiO_2–SiO_2 thin films by XPS and ab initio calculations. *Appl. Surf. Sci.*, 510:145056, 2020. doi: 10.1016/j.apsusc.2019.145056

47. J. Svoboda, D. Holec, M. Popov, G. A. Zickler, and F. D. Fischer. Modelling of short-range ordering kinetics in dilute multicomponent substitutional solid solutions. *Philos. Mag.*, pages 1–20, 2020. doi: 10.1080/14786435.2020.1750097

48. M. N. Popov, T. Dengg, D. Gehringer, and D. Holec. Adsorption of H_2 on Penta-Octa-Penta graphene: Grand canonical monte carlo study. *C — Journal of Carbon Research*, 6(2):20, 2020. doi: 10.3390/c6020020

49. D. Gehringer, T. Dengg, M. N. Popov, and D. Holec. Interactions between a H_2 molecule and carbon nanostructures: A DFT study. *C — Journal of Carbon Research*, 6(1):16, 2020. doi: 10.3390/c6010016

50. Y. W. Sun, D. Holec, D. Gehringer, O. Fenwick, D. J. Dunstan, and C. J. Humphreys. Unexpected softness of bilayer graphene and softening of A-A stacked graphene layers. *Phys. Rev. B Condens. Matter*, 101(12):125421, 2020. doi: 10.1103/PhysRevB.101.125421

51. D. Holec, P. Dumitraschkewitz, D. Vollath, and F. D. Fischer. Surface energy of au nanoparticles depending on their size and shape. *Nanomaterials (Basel)*, 10(3):484, 2020. doi: 10.3390/nano10030484

52. S. Mirzaei, M. Alishahi, P. Souček, J. Ženíšek, D. Holec, N. Koutná, V. Buršíková, M. Stupavská, L. Zábranský, F. Burmeister, B. Blug, Z. Czigány, K. Balázsi, R. Mikšová, and P. Vašina. The effect of chemical composition on the structure, chemistry and mechanical properties of magnetron sputtered W-B-C coatings: Modeling and experiments. *Surf. Coat. Technol.*, 383:125274, 2020. doi: 10.1016/j.surfcoat.2019.125274

53. M. Friák, D. Lago, N. Koutná, D. Holec, T. Rebok, and M. Šob. Multi-phase ELAStic aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. *Comput. Phys. Commun.*, 247:106863, 2020. doi: 10.1016/j.cpc.2019.106863

54. N. Koutná, R. Hahn, J. Zálešák, M. Friák, M. Bartosik, J. Keckes, M. Šob, P. H. Mayrhofer, and D. Holec. Point-defect engineering of MoN/TaN superlattice films: A first-principles and experimental study. *Mater. Des.*, 186:108211, 2020. doi: 10.1016/j.matdes.2019.108211

55. F. Guo, D. Holec, J. Wang, S. Li, and Y. Du. Impact of v, hf and si on oxidation processes in Ti–Al–N: Insights from ab initio molecular dynamics. *Surf. Coat. Technol.*, 381:125125, 2020. doi: 10.1016/j.surfcoat.2019.125125

56. S. Zöhrer, M. Golizadeh, N. Koutná, D. Holec, A. Anders, and R. Franz. Erosion and cathodic arc plasma of Nb–Al cathodes: composite versus intermetallic. *Plasma Sources Sci. Technol.*, 29 (2):025022, 2020. doi: 10.1088/1361-6595/ab5e32

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4. **D. Holec, D. Gehringer, M.N. Popov, T. Leiner: "Hydrogen adsorption on graphene-based materials" (invited oral). *ICCCEBH 2022 (4th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina)*, Sarajevo, Bosna and Herzegovina, June 30–July 2, 2022.**

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45. D. Holec, L. Zhou, and P.H. Mayrhofer: "Predictive power of electron energy loss spectra modelled by first principles " (oral). *ICMCTF 2014 (41st International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 28–May 2, 2014.

46. S. Zhang, D. Holec, W.Y. Fu, C.J. Humphreys, P.H. Mayrhofer, and M.A. Moram: "Ab initio evaluation of the potential use of Sc-based III-nitrides in optoelectronics" (poster). *ICMCTF 2014 (41st International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 28–May 2, 2014.

47. **D. Holec: "What does a bunch of atoms reveal about behaviour of real materials?" (invited oral). *60. Metallkunde-Jubiläumskolloquium*, Lech am Arlberg, Austria, April 23–25, 2014.**

48. **D. Holec, M. Friák, A. Dlouhý, and J. Neugebauer: "Point defects in NiTi-based alloys" (invited oral). *The Czech-Japanese Workshop on High- Temperature Intermetallics*, Brno, Czech Republic, April 13–16, 2014.**

49. L. Zhou, D. Holec, M. Bartosik, F. Körmann, B. Grabowski, J. Neugebauer, and P.H. Mayrhofer: "Structural stability and thermodynamics of CrN magnetic phases from first principles" (poster). *ViCoM workshop (From Electrons to Phase Transitions)*, Vienna, Austria, February 26–28, 2014.

50. **D. Holec: "Alloying trends from first principles – A case study of ternary and multinary nitrides" (invited oral). *Nanotek 2013*, Las Vegas, USA, December 2–4, 2013.**

51. D. Holec, D. Legut, S. Mayer, and H. Clemens: "Interplay between chemical disorder and Mo content on mechanical stability of cubic body centred TiAl phase" (oral). *Intermetallics 2013*, Kloster Banz, Germany, September 30–October 4, 2013.

52. D. Holec, J. Keckes, P. Wagner, F. Tasnádi, M. Friák, J. Neugebauer, and P.H. Mayrhofer: "Texture dependent elastic constants of polycrystalline Zr–Al–N predicted by *ab initio* calculations" (oral). *ICMCTF 2013 (40th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 29–May 3, 2013.

53. D. Holec, L. Zhou, R. Rachbauer, and P.H. Mayrhofer: "First principles study of alloying trends in Ti–Al–N and Cr–Al–N systems" (poster). *ICMCTF 2013 (40th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 29–May 3, 2013.

54. D. Holec: "Texture influence on elastic constants of nitride alloys – A multiscale approach" (oral). *Max-Planck-Institut für Eisenforschung*, Düsseldorf, Germany, March 27, 2013.

55. **D. Holec, M. Hartmann, O. Paris, and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes; A multi-method density functional theory and monte carlo study" (invited oral). *84th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM)*, Novi Sad, Serbia, March 18–22, 2013.**

56. D. Holec, L. Zhou, R. Rachbauer, and P.H. Mayrhofer: "Alloying trends in Ti–Al–N and Cr–Al–N hard coatings" (oral). *Special Symposium on Simlation Activities at Montanuniversität*, Leoben, Austria, January 15, 2013.

57. **D. Holec: "Alloying Trends from First Principles: How Well Can We Do?" (invited oral). *Materials between Scientific Fields*, Brno, Czech Republic, November 15–16, 2012.**

58. D. Holec, R. Rachbauer, L. Zhou and P.H. Mayrhofer: "Calculational study of alloying effects in Ti–Al–N-based protective hard coatings" (oral). *ECCOMAS 2012 (6th European Congress on Computational Methods in Applied Sciences and Engineering)*, Vienna, Austria, September 10–14, 2012.

59. D. Holec, R. Rachbauer, L. Zhou and P.H. Mayrhofer: "Computer aided understanding and design of protective hard coatings by alloying" (oral). *ECNF 2012 (European Conference on Nanofilms)*, Ancona, Italy, June 17–22, 2012.

60. D. Holec and P.H. Mayrhofer: "Do nitride alloys exhibit Vegard's-like linear behaviour?" (oral). *ICMCTF 2012 (39th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 24–27, 2012.

61. D. Holec P. Wagner, M. Friák, and P.H. Mayrhofer: "Elasticity in binary and ternary transition metal nitrides" (poster). *ICMCTF 2012 (39th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 24–27, 2012.

62. D. Holec, M. Hartmann, M. Todt, F.D. Fischer, F.G. Rammerstorfer, D. Vollath and P.H. Mayrhofer: "Size-dependent surface properties of nanoparticles: An atomistic study" (oral). *58. Metallkunde-Kolloquium*, Lech am Arlberg, Austria, April 16–18 2012.

63. D. Holec: "Computer-aided modelling ranging from quantum, via atomistic to continuum level is used to support and interpret experimental observations, as well as to explore new basic-research areas" (poster). *WerWasWo*, Leoben, Austria, March 12–23, 2012.

64. D. Holec, M. Friák, A. Dlouhý and J. Neugebauer: "Ab initio study of pressure-induced structural transitions in NiTi: The unexpected appearance of hysteresis" (oral). *1st Austrian-German Workshop on Computational Materials Design*, Kramsach, Austria, January 24–26 2012.

    D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Modelling of electron energy loss near edge structures of alloys" (oral). *Max Planck Institut für Eisenforschung.* Düsseldorf, Germany, November 29, 2011.

65. D. Holec, P. Wagner and P.H. Mayrhofer: "Elasticity in binary and ternary transition metal nitrides" (poster). *Euromat 2011*, Montpellier, France, September 12–16 2011.

66. D. Holec, M. Friák, A. Dlouhý and J. Neugebauer: "Ab initio study of pressure-induced structural transitions in NiTi" (oral). *Euromat 2011*, Montpellier, France, September 12–16 2011.

67. **D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Modelling of electron energy near edge structures of alloys – How well can we do?" (invited oral). *International Conference on Electron Nanoscopy*, Hyderabad, India, July 6–8 2011.**

68. D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Electron energy loss near edge structures of AlN-based ternary thin films" (oral). *E-MRS Spring Meering*, Nice, France, May 9–13, 2011.

69. D. Holec, R. Rachbauer, L. Chen, L. Wang, D. Luef and P.H. Mayrhofer: "Phase stability and electronic structure of Ti-Al-N, Zr-Al-N and Hf-Al-N" (oral). *E-MRS Spring Meering*, Nice, France, May 9–13, 2011.

70. D. Holec, R. Rachbauer, and P.H. Mayrhofer: "Phase stability and electronic structure of Ti-Al-N, Zr-Al-N and Hf-Al-N" (oral). *SIMNET Symposium*, Graz, Austria,May 2, 2011.

71. D. Holec, M.A. Hartmann, O. Paris and P.H. Mayrhofer: "Structure, surface energy and stability of carbon fullerenes" (poster). *ISSC-18 (Interdisciplinary Surface Science Conference)*, Warwick, United Kingdom, April 1–4, 2011.

72. R. Rachbauer, D. Holec, M. Lattemann, L. Hultman and P.H. Mayrhofer: "Electronic origin of structure and mechanical properties in Y and Nb alloyed Ti–Al–N thin films" (poster). *ISSC-18 (Interdisciplinary Surface Science Conference)*, Warwick, United Kingdom, April 1–4, 2011.

73. D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Towards reliable modelling of ELNES of $Al_xGa_{1-x}N$ and other AlN based ternary alloys" (poster). *MSM-XVII (Microscopy of Semiconducting Materials)*, Cambridge, United Kingdom, April 1–4, 2011.

74. D. Holec: "Structural and electronic properties of alloys" (oral). *Seminar at the University of Linköping.* Linköping, Sweden, October 27, 2010.

75. D. Holec, M. Hartmann, O. Paris and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes" (oral). *27th Max Born Symposium on Multiscale Modeling of Real Materials*, Wroclaw, Poland, September 18–20, 2010.

76. D. Holec, M. Hartmann, O. Paris and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes" (oral). *MSMF-6 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 28–30, 2010.

77. D. Holec, R. Rachbauer and P.H. Mayrhofer: "Phase stability and electronic structure of Ti-Al-N, Zr-Al-N and Hf-Al-N" (oral). *MSMF-6 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 28–30, 2010.

78. D. Holec, R. Rachbauer, D. Kiener, P.H. Mayrhofer and C.J. Humphreys: "Towards reliable modelling of electron energy loss near edge structure of ternary alloys" (poster). *MSMF-6 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 28–30, 2010.

79. D. Holec, M. Hartmann, F.G. Rammerstorfer, O. Paris, F.D. Fischer and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes" (oral). *ICMCTF 2010 (37th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 26–30, 2010.

80. D. Holec, F. Rovere, P.H. Mayrhofer and P. Barna: "Pressure dependent stability of cubic and wurtzite phases within the TiN-AlN and CrN-AlN systems" (poster). *ICMCTF 2010 (37th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 26–30, 2010.

81. D. Holec, R. Franz, M.A. Moram and P.H. Mayrhofer: "The Bk phase: a new player on the stage (Phase stability of ternary nitrides)" (oral). *4th Surface Engineering Workshop Leoben–Aaachen*, Aachen, Germany, March 15–16, 2010.

82. D. Holec, R. Franz, P.H. Mayrhofer and C. Mitterer: "Phase stability and electronic structure of the Ti-Al-N and Nb-Al-N pseudo-binary systems" (oral). *CMMP09 (Condensed Matter and Materials Physics 2009)*, Warwick, UK, December 15–17, 2009.

83. D. Holec, P.H. Mayrhofer and C.J. Humphreys: "Ab inito calculations of electron energy loss near edge structure of ternary alloys" (poster). *CMMP09 (Condensed Matter and Materials Physics 2009)*, Warwick, UK, December 15–17, 2009.

84. D. Holec and P.H. Mayrhofer: "First principles studies on Ti-Al-N and Nb-Al-N" (oral). *Euromat 2009*, Glasgow, UK, September 7–10, 2009.

85. D. Holec, M. Petrov, L. Lymperakis, C.J. Humphreys and J. Neugebauer: "Theoretical study of strain effects on ELNES and electronic structure of AlGaN" (poster). *MRS Fall meeting 2008*, Boston, USA, December 1–5, 2008.

86. D. Holec and C.J. Humphreys: "Ab initio calculations of electron energy loss near edge structure of ternary alloys: III-nitrides" (oral). *SP-SSM 2008 (International Symposium on Structure-Property Relationships in Solid State Materials)*, Nantes, France, June 29–July 3, 2008.

87. D. Holec and C.J. Humphreys: "Ab initio calculations of electron energy loss near edge structure of ternary alloys: AlGaN" (poster). *TMCS workshop (Theory, Modelling and Computational Methods for Semiconductor Materials and Nanostructures)*, Manchester, UK, January 31–February 1, 2008.

88. D. Holec and C.J. Humphreys: "Modelling of threading dislocations reduction in GaN" (oral). *UKNC meeting*, Glasgow, UK, January 9–10, 2008.

89. D. Holec and C.J. Humphreys: "A theoretical study of ELNES spectra of $Al_xGa_{1-x}N$ using Wien2k and Telnes" (poster). *Autumn School on Materials Science and Electron Microscopy 2007*, Berlin, Germany, October 8–11, 2007.

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91. D. Holec, P.M.F.J. Costa, P.D. Cherns and C.J. Humphreys: "Detailed theoretical study of ELNES spectra of $Al_xGa_{1-x}N$ using Wien2k and Telnes programs" (poster). *Wien2k workshop*, Singapore, July 6–9, 2007.

92. D. Holec, P.M.F.J. Costa, P.D. Cherns and C.J. Humphreys: "Detailed theoretical study of ELNES spectra of $Al_xGa_{1-x}N$ using Wien2k and Telnes programs" (oral). *ICMAT 2007 (International Conference on Materials for Advanced Technologies)*, Singapore, July 1–6, 2007.

93. D. Holec and C.J. Humphreys: "Critical thickness calculations for non-polar InGaN/GaN systems" (oral). *MSMF-5 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 27–29, 2007.

94. D. Holec and C.J. Humphreys: "On properties of dislocations in wurtzite materials" (oral). *Workshop on Nitride based nanostructures*, Berlin, Germany, February 6–8, 2007.

95. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "Critical thickness calculations for $In_xGa_{1-x}N$/GaN" (oral). *EW3NS (European Workshop on III-Nitride Semiconductor Materials and Devices)*, Heraklion, Crete, Greece, September 18–20, 2006.

96. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "Critical thickness calculations for $In_xGa_{1-x}N$/GaN" (oral), *5-IWMCG (5th International Workshop on Modelling in Crystal Growth)*, Bamberg, Germany, September 10–13, 2006.

97. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "The effect of the hexagonal symmetry on critical thickness calculations for $In_xGa_{1-x}N$/GaN" (poster), *Junior–Euromat 2006*, Lausanne, Switzerland, September 4–8, 2006.

98. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "Misfit dislocations – theory and experiment" (oral). *UKNC meeting*, Sheffield, UK, July 4, 2006.

99. D. Holec and A. Dlouhý: "Stress redistributions and their impact on the precipitation in microstructures" (oral). *Applied Mechanics 2005*, Hrotovice, Czech Republic, March 29–April 1, 2005.

100. D. Holec and A. Dlouhý: "Properties of low-angle dislocation boundaries in precipitation hardened crystals" (poster). *Junior–Euromat 2004*, Lausanne, Switzerland, September 6–9, 2004.

101. D. Holec and A. Dlouhý: "Stability and motion of low-angle dislocation boundaries in precipitation hardened crystals" (oral). *MSMF-4 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 23–25, 2004.