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Academic grade **Dr. rer. nat.**
Date of birth 19.10.1974
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Academic Education

10.1995 – 07.2001 Study at the Physics Institute of Humboldt-University, Berlin
14. 04. 1998 Prediploma in Mathematics at the Humboldt-University, Berlin
14. 07. 2000 Master of Philosophy at Loughborough University, UK
27. 07. 2001 Diploma in Physics at the Humboldt-University, Berlin
23.09. 2005 Promotion in Physics (Dr. rer. nat.) at Humboldt-University, Berlin
Topic: “Many-body effects in the Kondo-lattice model”

Professional Career

11.2003 – 05.2005 Research Assistant at the Physics Institute of Humboldt-University, Berlin
05.2005 – 03.2006 Research Assistant at the Max-Planck-Institut für Eisenforschung GmbH
Since 04.2006 Head of the group „Computational Phase Studies“ at the Max-Planck-Institut für Eisenforschung GmbH
Since 10.2008 Head of the Advanced Study Group “Modelling” at the Interdisciplinary Center for Advanced Materials Simulations (ICAMS) at Ruhr-University Bochum
Since 08.2021 Acting head of the division “Materials Informatics” (FB6.4) of Bundesanstalt für Materialforschung und -prüfung (BAM)

Honours, Awards & Memberships

02.1998 – 03.2001 Fellow of „Studienstiftung des dt. Volkes“ (Study grant)
04.2001 – 10.2003 Fellow of „Friedrich-Naumann-Stiftung“ (Promotion grant)
05.2005 – 03.2006 Research fellow of the Max-Planck society

Publications

a) Publications in peer-reviewed scientific journals

- [1] T. Hickel, B. Grabowski, F. Körmann, J. Neugebauer: *Advancing density functional theory to finite temperatures: methods and applications in steel design*, Journal of Physics: Condensed Matter 24 (2011) 053202
- [2] C. Freysoldt, B. Grabowski, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti, C. G. Van de Walle: *First-principles calculations for point defects in solids*, Review of Modern Physics 86 (2014) 253
- [3] B. Dutta, A Cakir, C. Giacobbe, A. Al-Zubi, T. Hickel, M. Acet and J. Neugebauer: *Ab initio Prediction of Martensitic and Intermartensitic Phase Boundaries in Ni-Mn-Ga*, Phys. Rev. Lett. 116, 025503 (2016).
- [4] I. Stockem, A. Bergmann, A. Glensk, T. Hickel, F. Körmann, B. Grabowski, J. Neugebauer, B. Alling: *Anomalous Phonon Lifetime Shortening in Paramagnetic CrN Caused by Spin-Lattice Coupling: A Combined Spin and Ab Initio Molecular Dynamics Study*, Phys. Rev. Lett. 121, 125902 (2018).
- [5] H.I. Sözen, S. Ener, F. Maccari, K.P. Skokov, O. Gutfleisch, F. Körmann, J. Neugebauer, T. Hickel, *Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams*, Phys. Rev. Mater. 3, 084407 (2019).
- [6] J. Janssen, S. Surendralal, Y. Lysogorskiy, M. Todorova, T. Hickel, R. Drautz, J. Neugebauer, *pyiron: An integrated development environment for computational materials science*, Comp. Mater. Sci. 163, 24-36 (2019).
- [7] A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer, J. Neuhaus, K. Hradil, W. Petry, M. Leitner: *Phonon Lifetimes Throughout the Brillouin Zone at Elevated Temperatures from Experiment and ab initio*, Phys. Rev. Lett. 123, 235501 (2019).
- [8] S. Mu, R. Olsen, B. Dutta, L. Lindsay, G.D. Samolyuk, T. Berlijn, E.D. Specht, K. Jin, H. Bei, T. Hickel, B.C. Larson and G.M. Stocks: *Unfolding the complexity of phonon quasi-particle physics in disordered materials*, npj Comput. Mater., 6, 4 (2020).
- [9] X. Zhang, H. Wang, T. Hickel, J. Rogal, Y. Li, J. Neugebauer: *Mechanism of collective interstitial ordering in Fe-C alloys*, Nature Materials 19, 849 (2020).
- [10] H. Zhao, P. Chakraborty, D. Ponge, T. Hickel, B. Sun, C.-H. Wu, B. Gault, D. Raabe: *D. Hydrogen trapping and embrittlement in high-strength Al alloys*. Nature, 602 (2022) 437-441.

b) Other publications:

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c) Patents:

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