Research Profile Frauenheim Thomas

General data

Name	Frauenheim Thomas, Prof. Dr. rer. nat. habil.
Date/place of birth	28/12/1950, Penig
Children	Sandra (43), Michael (40)
Affiliation	28359 Bremen, BCCMS, University of Bremen, Am Fallturm 1
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Academic education / degrees

1969 - 1973	Undergraduate study of physics at Technical University Dresden with specialization (Diploma in 1973) in theoretical solid state physics
1973 - 1976	Research fellow (PhD); Technical University Dresden in the Theoretical Physics Department; Supervisor Prof. Dr. Gerd Röpke (Dr. rer. nat. in 1976 Thesis: *Phase transitions in multi-band Hubbard-models at various band filling*)
1983	Habilitation in Theoretical Physics; Technical University Dresden, Mentor: Prof. Dr. Klaus Elk (Thesis: *Crystal field effects and magneto-elastic interactions in Rare Earth and Actinide intermetallic compounds*)

Professional career

1973 - 1976	Research assistant, Technical University Dresden, Theoretical Physics Department
1976 - 1982	Postdoctoral research fellow at Joint Institute for Nuclear Research – JINR-Dubna, USSR, Laboratory of Neutron Physics
1981	Visiting scientist, University of Neuchatel with Prof. Hans Beck
1981 - 1982	Head of the Inelastic Neutron Scattering Group at JINR in Dubna, USSR
1982 - 1998	Associate Professor at Technical University Chemnitz Head of research group *Atomistic simulations of complex materials*
1991 - present	Visiting scientist/professor at different Universities and Research Laboratories throughout the world, including: ETH-Zürich, University Tor-Vergata Rome, Universities of Kent, Exeter, St. Andrews, Glasgow, Oxford and Cambridge, Harvard University, Universities of Michigan, California and Nevada, Hongkong University, City-University of Hong Kong, Argonne National Laboratory
1998 - 2006	Chair Professor for Theoretical Physics, University of Paderborn
2006 - present	Chair Professor for Computational Material Science, Bremen Center for Computational Material Sciences, University of Bremen, retired, Honorary Contract until 2025. https://www.bccms.uni-bremen.de/cms/
2009 – present	Director of the German CECAM-node Multi-scale Modeling from 1-st Principles www.cecam-mm1p.de
2020 - present	Chair Professor at Computational Science Research Center (CSRC) Beijing and at Computational Science and Applied Research (CSAR) Institute Shenzhen, please see, https://www.csrc.ac.cn/en/people/faculty/181.html

Awards / scientific and editorial boards

1992	Distinguished visiting Professor at University of Athens, Ohio, USA
2004	Staudinger Dürrer Medaille, ETH-Zurich
2009 - present	CECAM board of directors, Director of CECAM-node cecam-mm1p.de (Multiscale modelling from first principles)
2009 – present	Scientific advisory board – Area of Excellence – *Modelling and simulation of emerging electronics*, University of Hongkong

2019	1000-Talent Award of China for Foreign Senior Scientist and Chair Professor at Computational Science Research Center (CSRC) Beijing and at Computational Science and Applied Research (CSAR) Institute Shenzhen, please see, https://www.csrc.ac.cn/en/people/faculty/181.html

Selected research topics and professional accomplishments

Development of highly efficient and chemically accurate quantum-mechanically based simulation methods/tools having advanced functionality for dynamic atomistic treatment of many-atom (1000´s) nanostructures in electronic ground and excited states. Application of these methods to fundamental and technological relevant problems in material science. The primary focus is to understand structure-property-function correlations of complex materials systems in physics, chemistry, biology and engineering and to study materials functions under working load.

2002 - 2010	Speaker and coordinator of the DFG Research Group FO-490 *Molecular mechanisms of retinal proteins: A combination of theoretical approaches*
2006 - 2013	Speaker and coordinator of the DFG Priority Program SPP-1243 – Quantum transport on the molecular scale
2009 – present	Organizer of numerous International CECAM Workshops, Tutorials and Heraeus-Schools in Physics on computational topics in materials science, physics and biochemistry, see: http://www.bccms.uni-bremen.de/en/events/

Most important 3rd- party funding (last five years): “Semiconductor Nanowires for Optoelectronics”, DFG FOR 1616, RO 3639/2-1, 4/2012 until 3/2018; “Multi-scale approach for prediction of electrical properties of carbon nanotube reinfor- ced polymers”, DFG, FR 2833/36-1, 1/2013 until 12/2015; “Vorhersagende multiskalen Modellierung und Strukturdesign von optischen Schutzschichten basierend auf amorphen ternären Metalloxiden”, BMBF Pluto+, 7/2014 until 6/2017; “Charge transport in molecular wires”, DFG, FR 2833/50-1; “Quantum transport at the molecular scale“ (SPP 1243) DFG FR2833/27-1/2/3 and DFG FR2833/28-1/2/3; Speaker of the Research and Training Group “Quantum-Mechanica Materials Modelling: QM^3” DFG-RTG:2247.

10 most important publications

1. M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, Th. Frauenheim, S. Suhai, G. Seifert, *Self-Consistent-Charge Density-Functional Tight-Binding Method for Simulations of Complex Materials Properties*. Phys. Rev. B, **58**, p. 7260, 1998.
2. D. Porezag, T. Frauenheim, T. Köhler, G. Seifert, and R. Kaschner, *Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon*, Phys. Rev. B, vol. **51**, p. 12947, 1995.
3. M. Elstner, P. Hobza, T. Frauenheim, S. Suhai, and E. Kaxiras, *Hydrogen bonding and stacking interactions of nucleic acid base pairs: a density-functional-theory based treatment,* J. Chem. Phys., vol. **114**, p. 5149, 2001.
4. M. Elstner, T. Frauenheim, E. Kaxiras, G. Seifert, and S. Suhai, *A self-consistent-charge density-functional tight-binding scheme for large biomolecules,* phys. stat. sol.(b), vol. **217/1**, p. 375, 2000.
5. Q. Cui, M. Elstner, E. Kaxiras, T. Frauenheim, and M. Karplus, *A QM/MM-Implementation of the Self-Consistent-Charge Density-Functional Tight-Binding Method with the CHARMM Force Field*, J. Phys. Chem. B, vol. **105**, p. 569, 2001.
6. T. Frauenheim, G. Seifert, M. Elstner, t.A. Niehaus et al. *Atomistic simulations of complex materials: ground-state and excited-state properties,* Journal Phys. Cond. Mat. **14**, 3015, 2002.
7. B. Aradi, B. Hourahine, T. Frauenheim, *DFTB+, a sparse matrix-based implementation of the DFTB method,* J. Phys. Chem. **A 111**, 5678, 2007.
8. G. Seifert, H. Terrones, M. Terrones, G. Jungnickel, T. Frauenheim, *Structure and electronic properties of MoS2 nanotubes,* Phys. Rev. Lett. **85**, 146, 2000.
9. P. Deak, B. Aradi, T. Frauenheim, E, Janzen, A. Gali*, Accurate defect levels obtained from the HSE06 range-separated hybrid functional,*Phys. Rev. B **81**, 153203, 2010.
10. A. Pecchia, A. di Carlo, T. Frauenheim, S. Sanna, R. Gutierrez, T. Frauenheim, *Incoherent electron-phonon scattering in octanethiols,*Nano Letters **4**, 2109, 2004.

ISI Web of Science: 622 refereed papers in international journals.

SCOPUS Research Profile: https://www.scopus.com/authid/detail.uri?authorId=7005494448

Google Scholar: https://scholar.google.com/citations?user=Z6cXcTEAAAAJ&hl=de