CURRICULUM VITAE

Ao.Univ.Prof. Dipl.-Ing. Dr.techn. Peter BLAHA

Born: 5 July 1955, Vienna, Austria
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Education: High School Diploma (Matura) 1974

Dipl.Ing. (Technische Chemie) Technische Universität Wien, 1980
Dr.techn., Technische Universität Wien, 1983
Docent (Habilitation) in Computational Chemistry 1992

Positions held:

Assistant, Inst. f. Technical Electrochemistry, TU Vienna 1980 -- 92
PostDoc, Louisiana State Univ., Baton Rouge, La, USA 1984 -- 1985
A.o.Professor, TU Vienna 1992 - present
Visiting scientist or Guest Professor at:
- Inst.f.Festkörperforschung, KFA Jülich (1986)
- University of Florida, Gainesville, USA (1988)
- Princeton University, USA (1999)
- University Santiago de Compostella, Spain (2000)
- Université du Maine, Le Mans, France (2005)

Awards: Kardinal Innitzer Award (1992)
Wiener Ingenieurpreis 2012

Research Interest:

- Ab-initio density-functional theory
- Development of the bandstructure code WIEN2k
- Physics and chemistry of inorganic materials, magnetism, structure
- theoretical spectroscopy (XPS, UPS, XES, XAS, EELS, IR, NMR, …)

Publications:

26 invited talks in the last 5 years;
302 publications in international journals;
H-index: 55
selected recent papers:

P.Blaha, K.Schwarz, G.K.H.Madsen, D.Kvasnicka, J.Luitz:
"WIEN2k: An Augmented Plane Wave plus Local Orbitals Program for Calculating Crystal Properties",
K.Schwarz, TU Wien, 2001 (ISBN 3-9501031-1-2)

G.K.H. Madsen, K. Schwarz, P. Blaha, D.J. Singh:
Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium
Physical Review B, 68 (2003), 125212 - 125217.

R. Laskowski, G.K.H. Madsen, P. Blaha, K. Schwarz:
"*Magnetic structure and electric-field gradients of uranium dioxide: An ab initio study*";
Physical Review B, **69** (2004), S. 140408(R).

I. Sergienko, V. Keppens, M. McGuire, R. Jin, J. He, S. Curnoe, B. Sales, P. Blaha, D.J. Singh, K. Schwarz, D. Mandrus:
"*Metallic "Ferroelectricity" in the Pyrochlore $Cd_2Re_2O_7$*";
Physical Review Letters, **92** (2004), S. 065501 - 065504.

R. Laskowski, P. Blaha, T. Gallauner, K. Schwarz:
"*Single-Layer Model of the Hexagonal Boron Nitride nanomesh on the Rh(111) surface*";
Physical Review Letters, **98** (2007), 106802.

F. Tran, R. Laskowski, P. Blaha, K. Schwarz:
"*Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional*";
Physical Review B, **75** (2007), 115131.

S. Berner, M. Corso, R. Widmer, O. Groening, R. Laskowski, P. Blaha, K. Schwarz, A. Goriachko, H. Over, S. Gsell, M. Schreck, H. Sachdev, T. Greber, J. Osterwalder:
"*Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer*";
Angewandte Chemie - International Edition, **46** (2007), 5115 - 5119.

M. Body, C. Legein, J. Buzare, G. Silly, P. Blaha, C. Martineau, F. Calvayrac:
"*Advances in Structural Analysis of Fluoroaluminates Using DFT Calculations of ^{27}Al Electric Field Gradients*";
Journal of Physical Chemistry A, **111** (2007), S. 11873 - 11884.

H. Dill, J. Lobo-Checa, R. Laskowski, P. Blaha, S. Berner, J. Osterwalder, T. Greber:
"*Surface Trapping of Atoms and Molecules with Dipole Rings*";
Science, **319** (2008), S. 1824.

F.Tran and P.Blaha:
"*Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential*",
Physical Review Letters 102, 226401(2009).

R. Laskowski, P. Blaha:
„*Understanding the $L_{2,3}$ x-ray absorption spectra of early 3d transition elements*",
Physical Review B 82, 205105(2010).

H. Hsu, P. Blaha, M. Cococcioni, R. Wentzcovitch:
“Spin-State Crossover and Hyperfine Interactions of Ferric Iron in $MgSiO_3$ Perovskite“,
Physical Review Letters 106, 118501 (2011).

E. Assmann, P. Blaha, R. Laskowski, K. Held, S. Okamoto, G. Sangiovanni:
"Oxide Heterostructures for Efficient Solar Cells";
Physical Review Letters, 110 (2013), 078701.

G. Parkinson, Z. Novotny, G. Argentero, M. Schmid, J. Pavelec, R. Kosak, P. Blaha, U. Diebold:
"*Carbon monoxide-induced adatom sintering in a Pd-Fe_{3}O_{4} model catalyst*";
Nature Materials, **12** (2013), 724 - 728.

X. Rocquefelte, K. Schwarz, P. Blaha, S. Kumar, J. van den Brink:
”Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide“;
Nature Comm. 4, (2013), 2511.

A. Tröster, W. Schranz, F. Karsai, P. Blaha:
"Fully Consistent Finite-Strain Landau Theory for High-Pressure Phase Transitions";
Physical Review X, 4 (2014), 031010.

R. Bliem, E. McDermott, P. Ferstl, M. Setvin, O. Gamba Vasquez, J. Pavelec, M. Schneider, M. Schmid, U. Diebold, P. Blaha, L. Hammer, G. Parkinson:
"Subsurface cation vacancy stabilization of the magnetite (001) surface";
Science, 346 (2014), 1215 - 1218.

H. Jiang, P. Blaha:
"*GW with linearized augmented plane waves extended by high-energy local orbitals*";
Physical Review B, **93** (2016), S. 115203.

R. Laskowski, P. Blaha:
"*NMR Shielding in Metals Using the Augmented Plane Wave Method*";
Journal of Physical Chemistry C, **119** (2015), S. 19390 - 19396.

K. Lejaeghere, P. Blaha, K. Schwarz et al.:
"*Reproducibility in density functional theory calculations of solids*";
Science, **351** (2016), S. aad3000.