

# CURRICULUM VITAE

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

**Born:** 5 July 1955, Vienna, Austria  
**Nationality:** Austria  
**Home Address:** Paulinensteig 34, A-1160 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 -  
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)

**Research Interest:**

- Ab-initio density-functional theory
- Development of the bandstructure code WIEN2k
- Physics and chemistry of inorganic materials, magnetism, structure
- Electric field gradients

**Publications:** More than 190 publications in international journals, 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. Nicolay, F. Reinert, S. Hüfner and P. Blaha:  
*Spin-orbit splitting of the L-gap surface state on Au(111) and Ag(111)*,  
Phys. Rev. B **65**, 033407 (2002)

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.

G. Grad, P. Blaha, K. Schwarz, W. Auwärter, T. Greber:  
*Density functional theory investigation of the geometric and spintronic structure of h-BN/Ni(111)  
in view of photoemission and STM experiments*  
Physical Review B, **68** (2003), 085404 - 085411.

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).

J. Schäfer, D. Schrupp, E. Rotenberg, K. Rossnagel, H. Koh, P. Blaha, R. Claessen:  
*"Electronic Quasiparticle Renormalization on the Spin Wave Energy Scale"*;  
Physical Review Letters, **92** (2004), S. 097205 - 097208.

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<sub>2</sub>Re<sub>2</sub>O<sub>7</sub>"*;  
Physical Review Letters, **92** (2004), S. 065501 - 065504.

J.M. Perez-Mato, M. Aroyo, A. Garcia, P. Blaha, K. Schwarz, J. Schweifer, K. Parlinski:  
*"Competing structural instabilities in the ferroelectric Aurivillius compound SrBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub>"*;  
Physical Review B, **70** (2004), 214111.

P. Blaha, K. Schwarz, P. Novak:  
*"Electric Field Gradients in Cuprates: Does LDA+U give the Correct Charge Distribution ?"*;  
International Journal of Quantum Chemistry, **101** (2005), 550 - 556.

J. Schäfer, M. Hoinkis, E. Rotenberg, P. Blaha, R. Claessen:  
*"Fermi surface and electron correlation effects of ferromagnetic iron"*;  
Physical Review B, **72** (2005), 155115.

I. Etxebarria, J.M. Perez-Mato, A. Garcia, P. Blaha, K. Schwarz, J. Rodriguez-Carvajal:  
*"Comparison of empirical bond-valence and first-principles energy calculations for a complex  
structural instability"*;  
Physical Review B, **72** (2005), 174108.