Tuturial: (*ab initio*)

Density Functional Calculations with FPLO

Manuel Richter (IFW Dresden)

FPLO: full-potential local-orbital code; http://www.fplo.de

100,000 FORTRAN lines; 100,000 C lines; 20 person years

here: basic handling of the code, no internal stuff

You will sit at the computer and solve tasks, 40 students at 20 computers assisted by 4 tutors:

band structure of Al; magnetic moment of Fe; magneto-crystalline anisotropy of Co; magnetic ground state of Ni_2

Electronic Structure:

LDA, LSDA, Tight Binding, DMFT

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A Local Density Approximation (LDA)

B Tight Binding Approximation (TB)

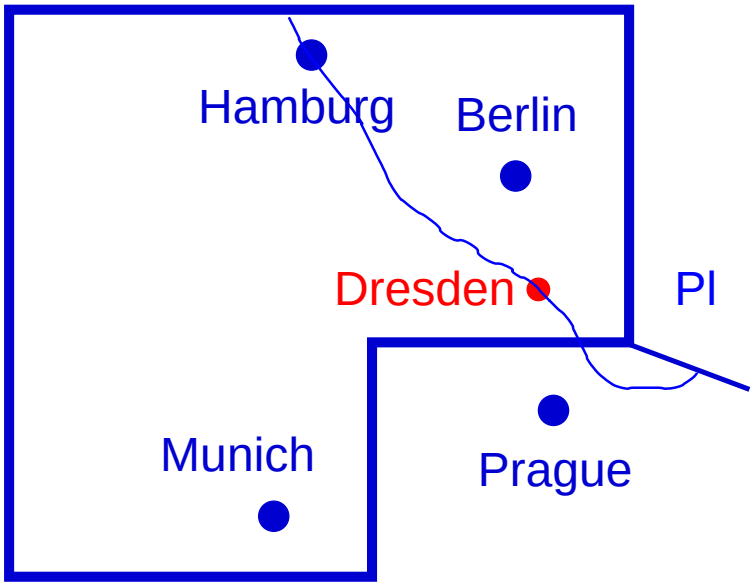
C Local Spin Density Approximation (LSDA)

D Applications and a Hint on Dynamical Mean Field Theory (DMFT)

Dresden: founded in 1206; flooded in 2002

500.000 inhabitants,

50.000 at University, 3 Max-Planck-Institutes, 3 Leibniz-Institutes



IFW: Solid State and Materials Res.

$\approx$ 450 employees, 65 staff scientists

Theoretical Solid State Physics

with 10 senior scientists,

3 postdocs, 6 PhD students, guests,

$\approx$ 300 CPUs

Recommended Literature:

LDA	H. Eschrig	*The Fundamentals of Density Functional Theory* EAGLE 2003, ISBN 3-937219-04-8
TB	J. Singleton	*Band Theory and Electronic Properties of Solids* Oxford University Press 2006, ISBN 0-19-850644-9
LSDA	S. Blundell	*Magnetism in Condensed Matter* Oxford University Press 2006, ISBN 0-19-850591-4
	J. Kübler	*Theory of Itinerant Electron Magnetism* Oxford University Press 2000, ISBN 0-19-850028-9
	M. Richter	*Band structure theory of magnetism in 3d-4f compounds* J. Phys. D: Applied Physics **31**, 1017–1048 (1998)
DMFT	A. Georges *et al.*	*Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions* Rev. Mod. Phys. **68**, 13–125 (1996)