VIRTUAL DESIGN OF QUANTUM MATERIALS

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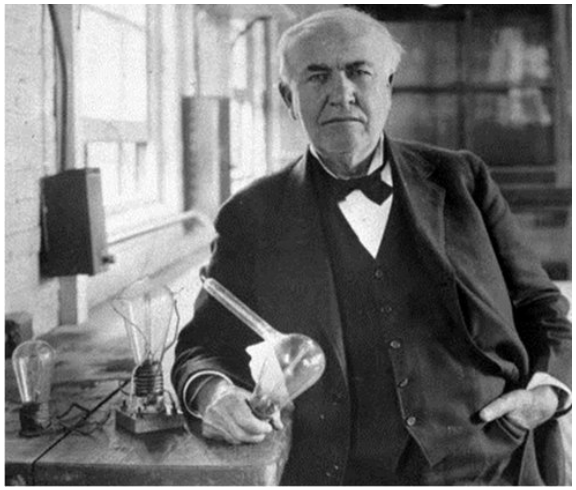
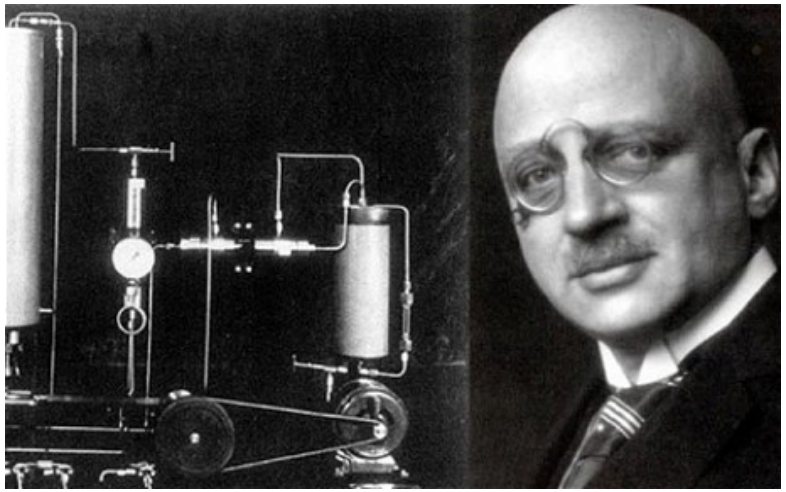
MATERIALS' DEVELOPMENT STILL EDISONIAN: INTUITION, SEARCHES, AND SERENDIPITY

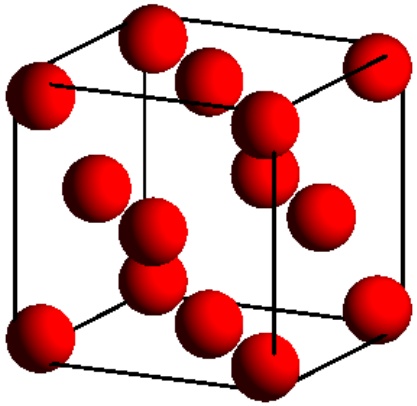
- Edison tested 3000 materials for his filament – settling on burned sewing thread.
- Haber–Bosch ammonia synthesis used osmium as catalyst. Mittasch (BASF) tested more than 22,000 materials to identify the iron-based catalyst which is still used today.





THEORY → MATERIAL PROPERTIES

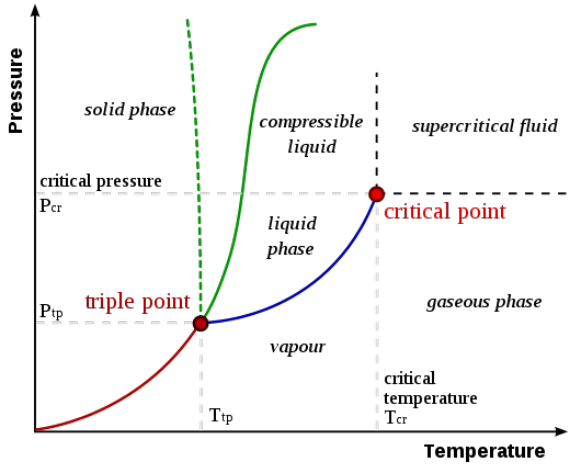
Structure



Calculation

Inverse Problem

Property



- Many possible approaches: multiscale modelling
- Electronic, magnetic, atomic properties of solids, surfaces, interfaces

KOHN SHAM – DENSITY FUNCTIONAL THEORY

- Standard Model in many Fields:
  Physics, Chemistry, Material Science, Biology, …
- Basic idea:

$$\left(\sum_i h_i + \sum_{i,j} U_{ij} \right) \Psi(\vec{r}_1, \ldots \vec{r}_N) = E \Psi(\vec{r}_1, \ldots \vec{r}_N)$$

- Mapping of the many-electron system on a system of non-interacting electrons described by an effective single-particle Hamiltonian

$$h\psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r})$$

METHOD DEVELOPMENT

www.flapw.de

fleur KKR*nano*

juRS **juDFT**

KKR*imp*

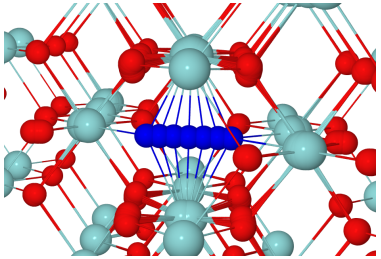
juNoLo KKR*susc*

juTiBi juSpinX

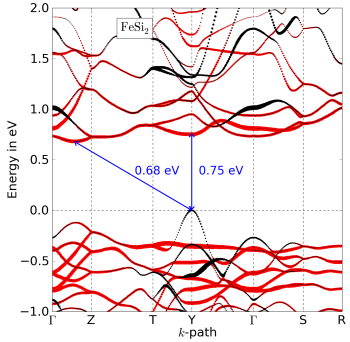
All-electron DFT:

- No element-specific pseudopotential
- Complex electronic structure
- Complex magnetism
- Topological states of matter
- Transport

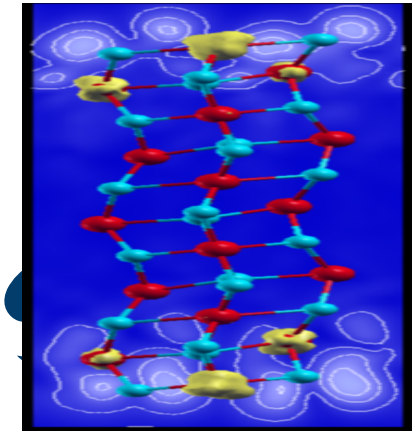
Atomic structure
Total energies
Forces



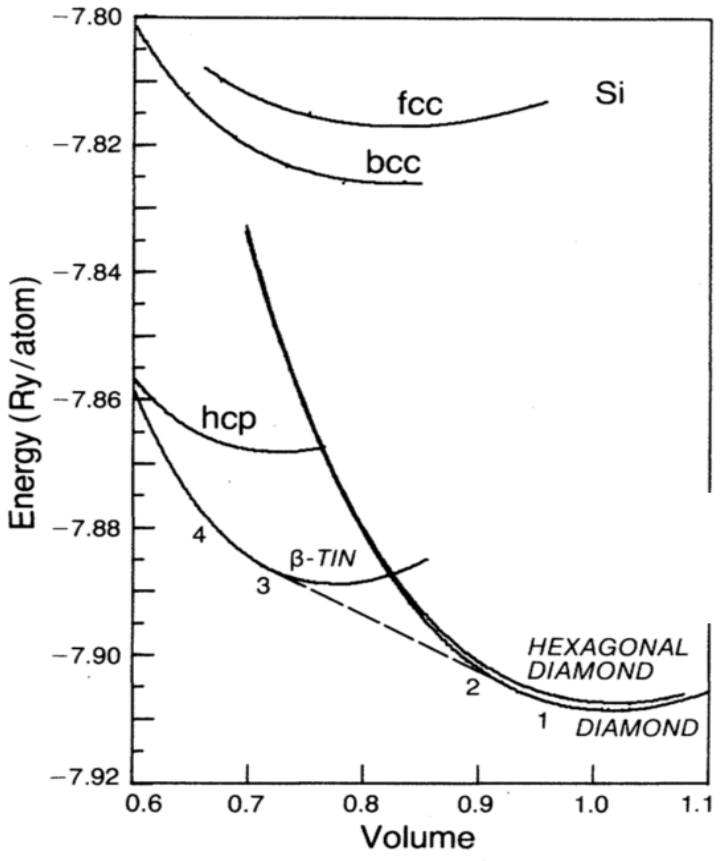
Electronic structure
Bandgaps
Bandstructures



Charge density
Surface states

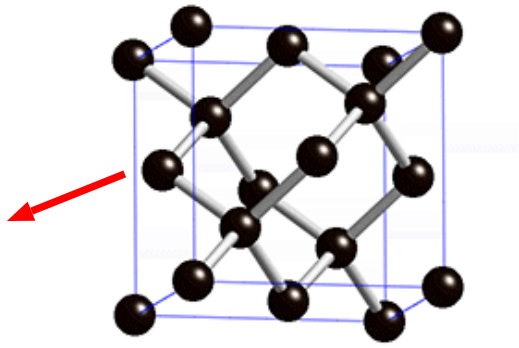


PREDICTIVE POWER OF DFT



Most simple example:

- Si bulk
- Correct volume, structure, transitions
- First-principles simulations



MAIN CHALLENGES

How to ensure data-quality:

- Different approximations for different properties
- Different approximations for different structures
- Different accuracy needed for different properties/structures

Data provenance:

- More important to store ‘recipe’ rather than final result
- Our data can easily be recreated

Managing workflows is of key importance

WHAT IS A WORKFLOW?

Technical:
A (Python) script defining, submitting and postprocessing DFT-computations

Workflows facilitate:

- Determination of complex materials properties from simple input of structures
- Key part of any high-throughput scheme
- Simple workflows act as building blocks for more sophisticated and larger workflows
- Way of providing expert knowledge to users
- Evolution of DFT codes into tools useable by non-expert users

THE WORKFLOW ENVIRONMENT

Requirements:

- Job management
- Data handling
- Data processing

- Extendable
- Open source

We need to store:

- Structures
- Parameters
- Codes, Computers
- Calculations
- Results

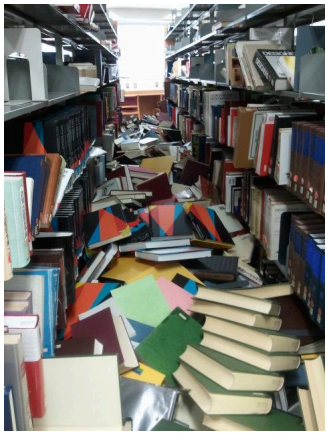
Automated Interactive Infrastructure and
Database for Computational Science

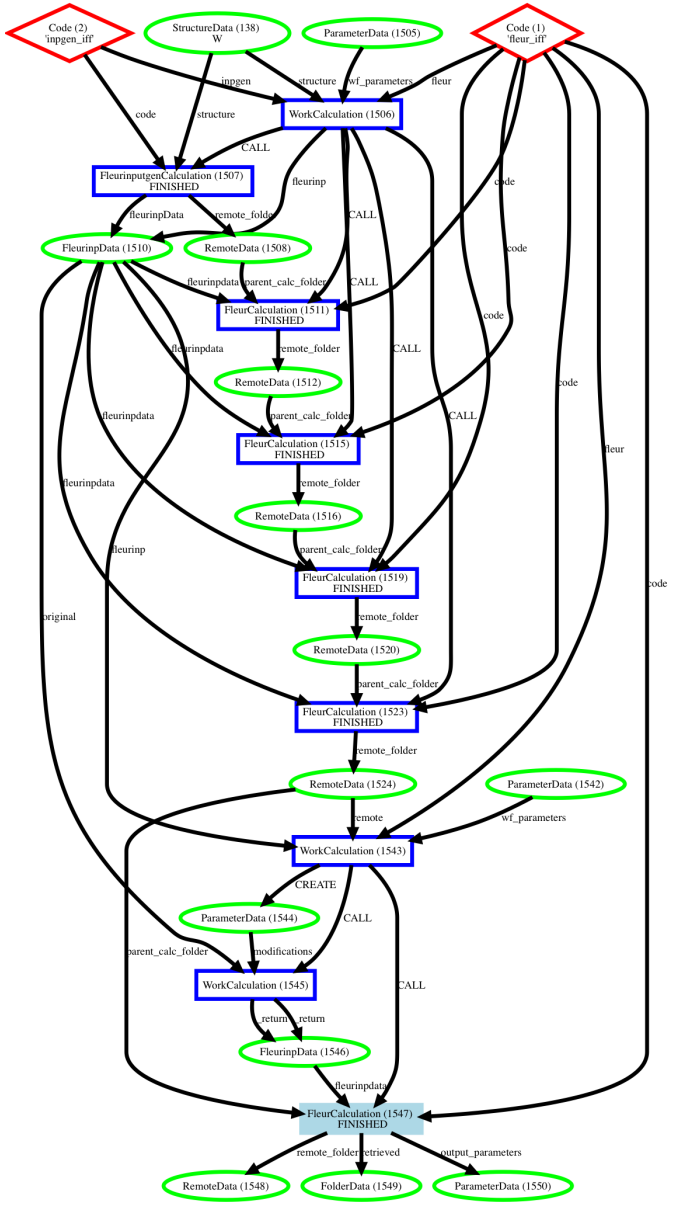
Main developers @EPFL:

G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (‘16)

NODE GRAPH OF CONVERGENCE WF

- Each node corresponds to database entry
- Full provenance of calculations and results
- Even most simple calculations generate a lot of data



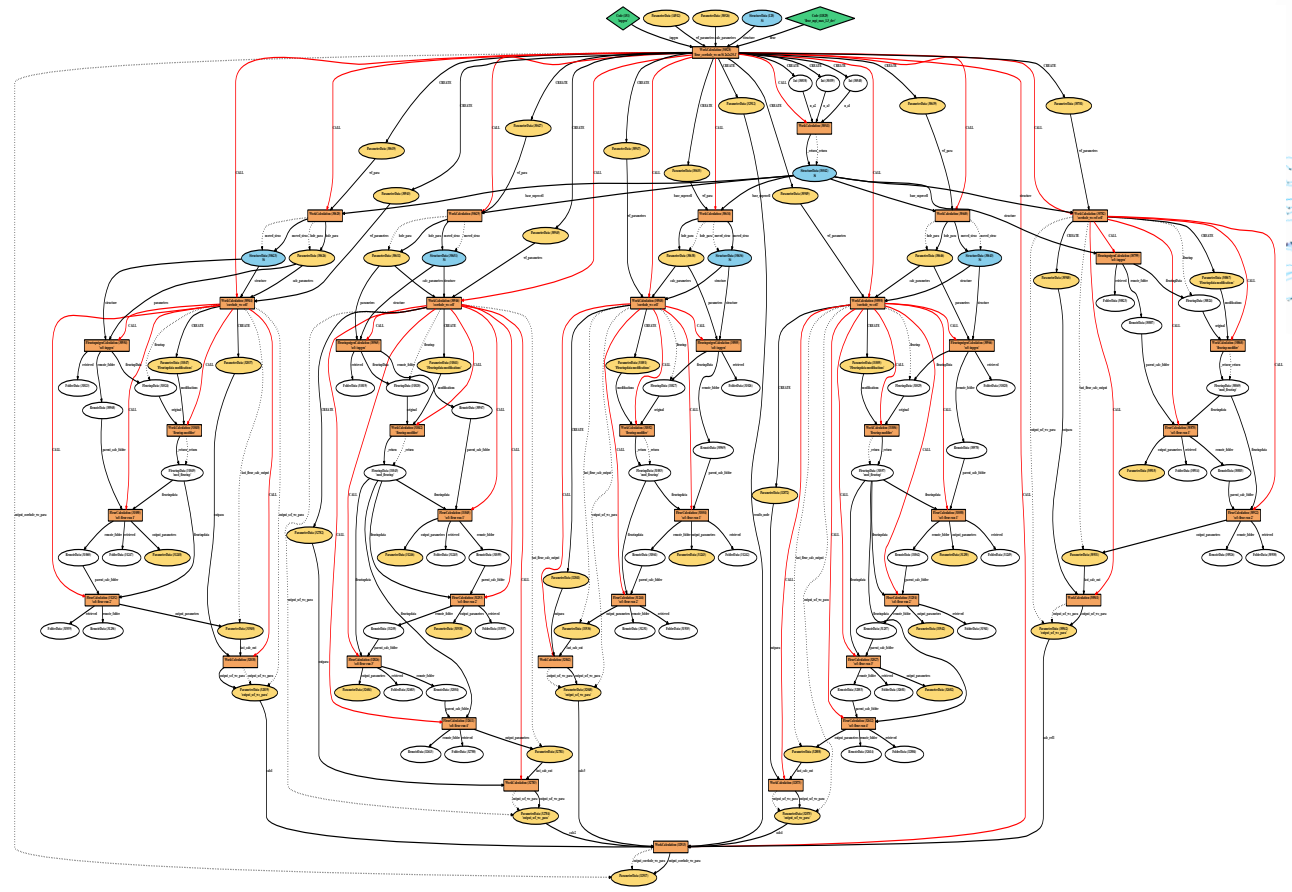


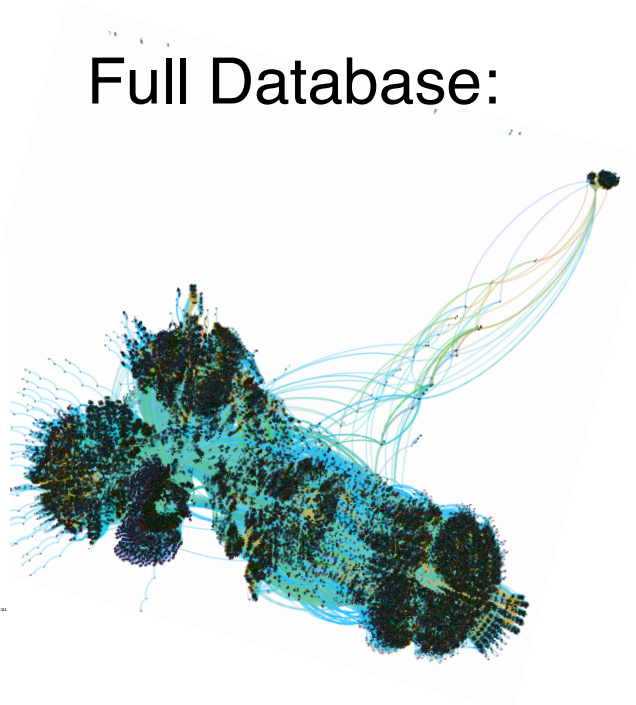
STRUCTURED DATABASE

AiiDA:

- Not a simple structure → property table
- Python tools for data analytics

Full Database:





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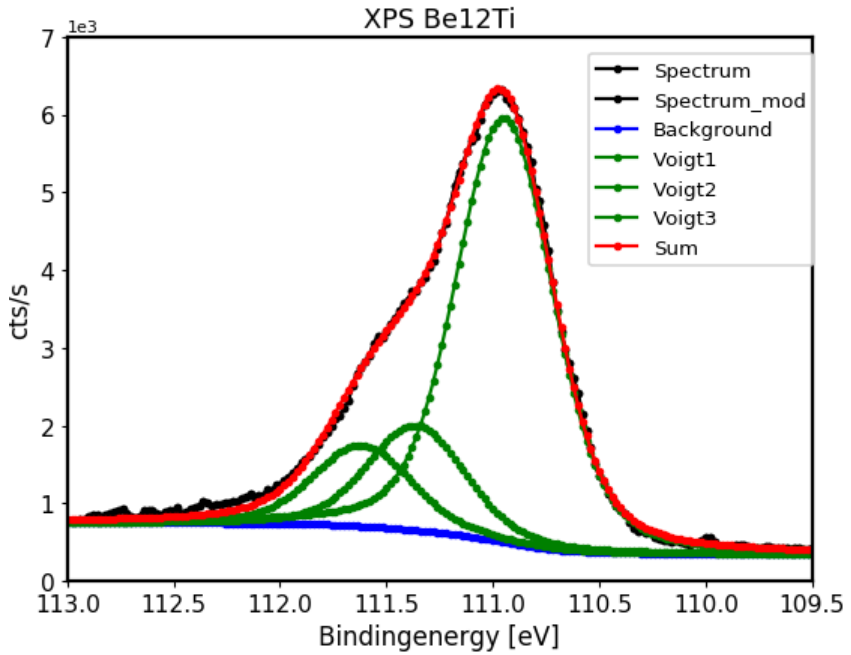
SIMULATION OF XPS DATA

Experiments (FZJ-IEK4):

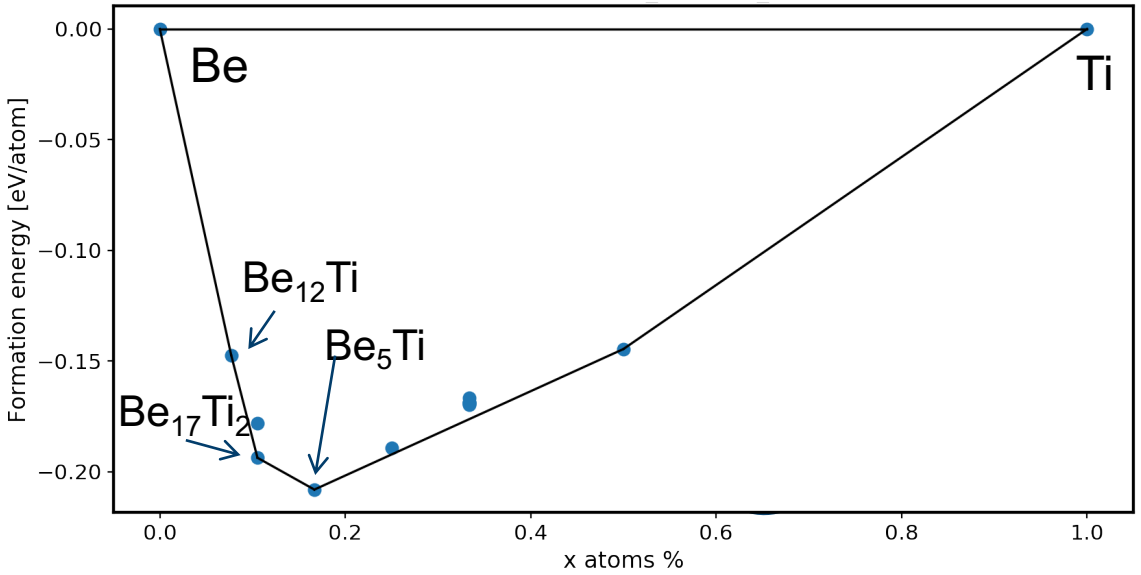
- XPS investigation of Beryllides
- Unclear details of spectrum $Be_{12}Ti$
- Three peaks?



N. Helfer, FZJ-IEK4, TU-Dortmund

1. Theoretical finding:

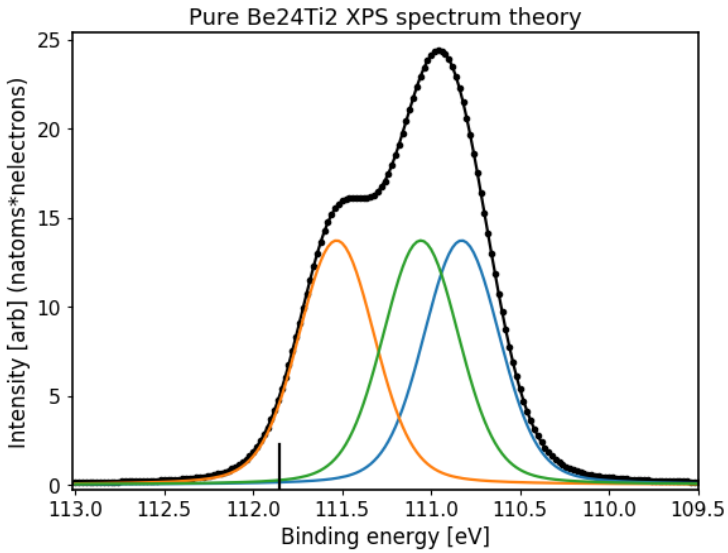
- Convex hull calculated
- Different structures possible



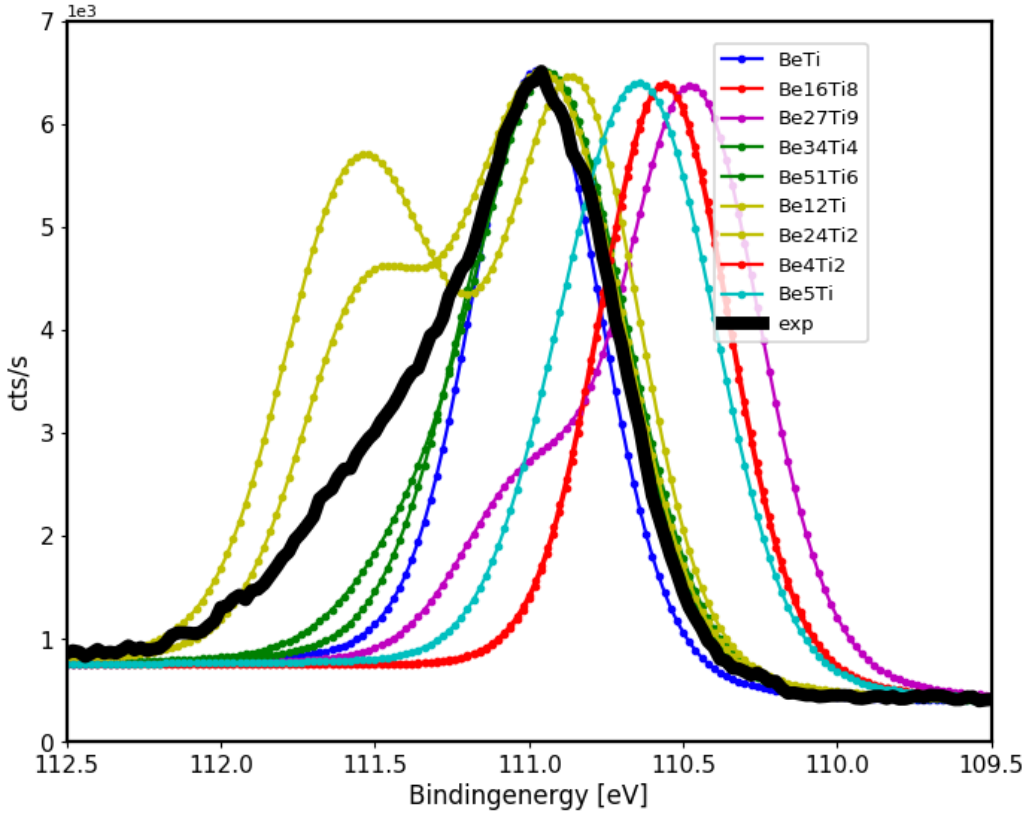
XPS DATABASE

Simulation of XPS spectra for all Be-Ti alloys:

- Binding energies of core-states
- Symmetry information for relative weights of peaks
- Superposition with peak-width



Nothing really fits!



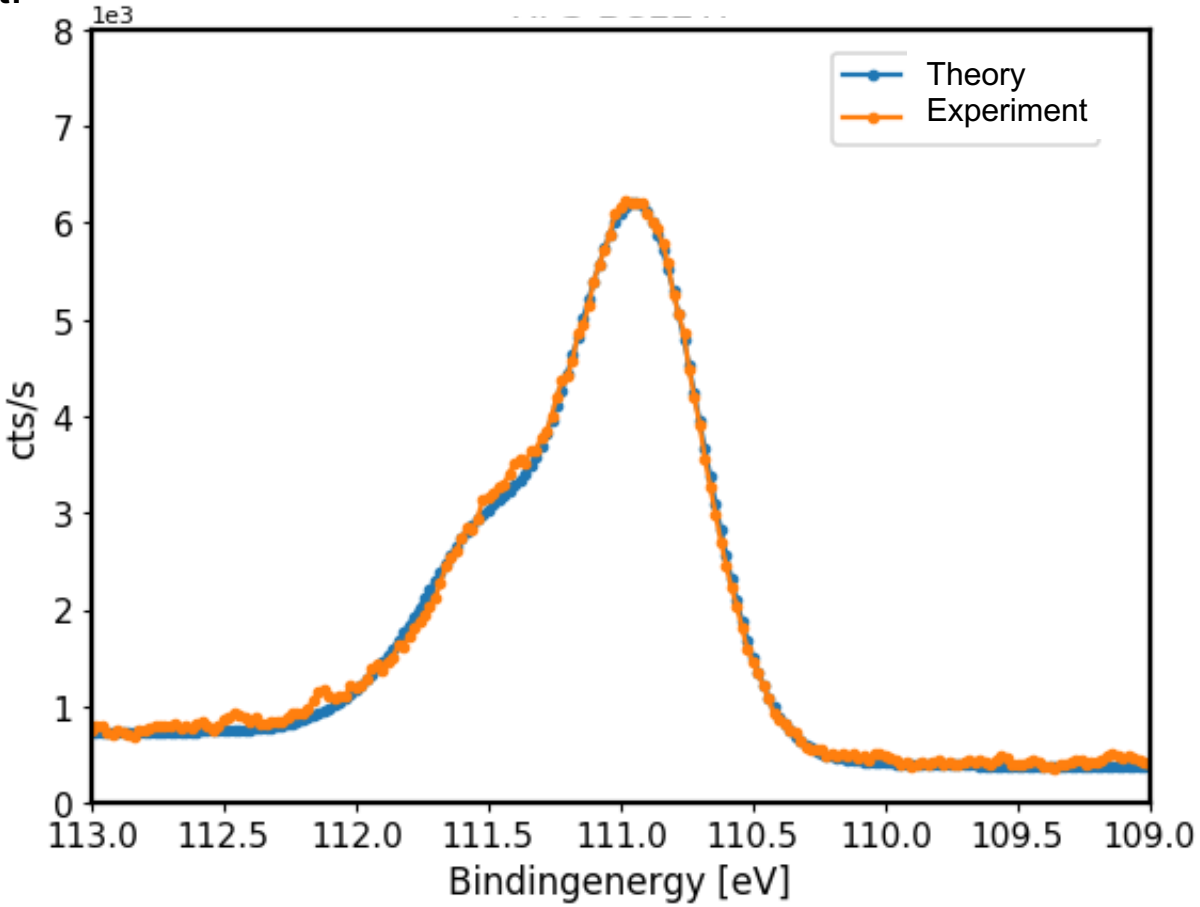
XPS DATABASE

- A mixture provides perfect fit:

  75% $Be_{12}Ti$ + 25% $Be_{17}Ti_2$

- Fit with 3-4 parameters:
  - Reference energy
  - Peak width
  - Relative concentration

- In agreement with experimental expectations/observations



APP FOR CORE-LEVEL SHIFT

jupyter Edit App

1 Visualization for Core-level spectra

Welcome! Here you can plot theoretical core-level spectra from the data in the database. This GUI just wraps some functionalities of the method 'plot_methods.plot_fleur_aiida.plot_spectra'. You can export the data or save the plot. Enjoy! Created @ PGI-1 by Jens Broeder

Nodes PK/UUID: 41983 41982 41981

Factors: e.g. 5.1 1 1 (space seperator # of factors has to be equal # of pks)

Emin [eV]: 109

Emax [eV]: 113

Energy grid... 0.020

fwhm_l [eV]: 0.10

fwhm_g [eV]: 0.60

Peakfunction t... e.g. voigt gaus lorentz pseudo-voigt (only one)

Download Data

Plot

```
WARNING: outputnode uuid: 6e87bb25-d07c-4c2f-9be5-e146c89bb5d5 (pk: 65836), states that workchain was not su
, check the results!
Material: Be4Ta2
WARNING: outputnode uuid: b07b18b0-2150-45a3-ad6e-4bc74cf77ec5 (pk: 65833), states that workchain was not su
, check the results!
Material: Be9Ta3
WARNING: outputnode uuid: 91c0cc9f-4758-4c53-8a9e-81f1071e220f (pk: 65830), states that workchain was not su
, check the results!
Material: Be17Ta2
{u'Be': {'1s1/2': [110.58513559265708,
                   110.48196818319055,
                   110.97176765661968,
                   110.4233986707561,
                   111.55940708347579,
                   111.06630964992608,
                   111.209057380928,
                   111.09462807132125]},
 u'Ta': {'4d5/2': [226.1200727699553,
                   226.1027026265919,
                   226.76010887979797,
                   227.22198594729 61],
         '4f5/2': [23.524019329788484,
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                   24.153426372926493,
                   24.61528595166682],
         '4f7/2': [21.42425830562279,
```

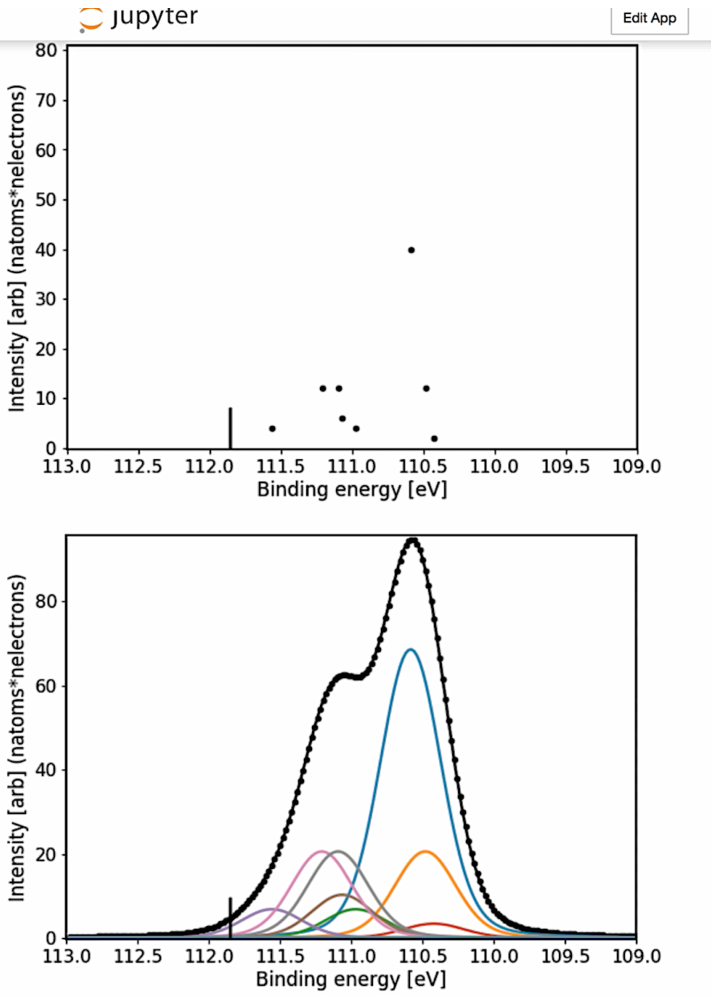

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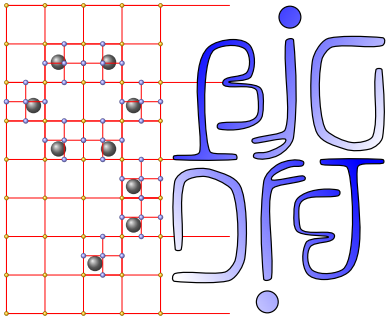
MATERIALS AT THE EXASCALE
A EUROPEAN CENTER OF EXCELLENCE IN HPC

MAX DRIVING THE EXASCALE TRANSITION

Flagship codes

QUANTUMESPRESSO

Yambo



siesta

www.flapw.de

fleur

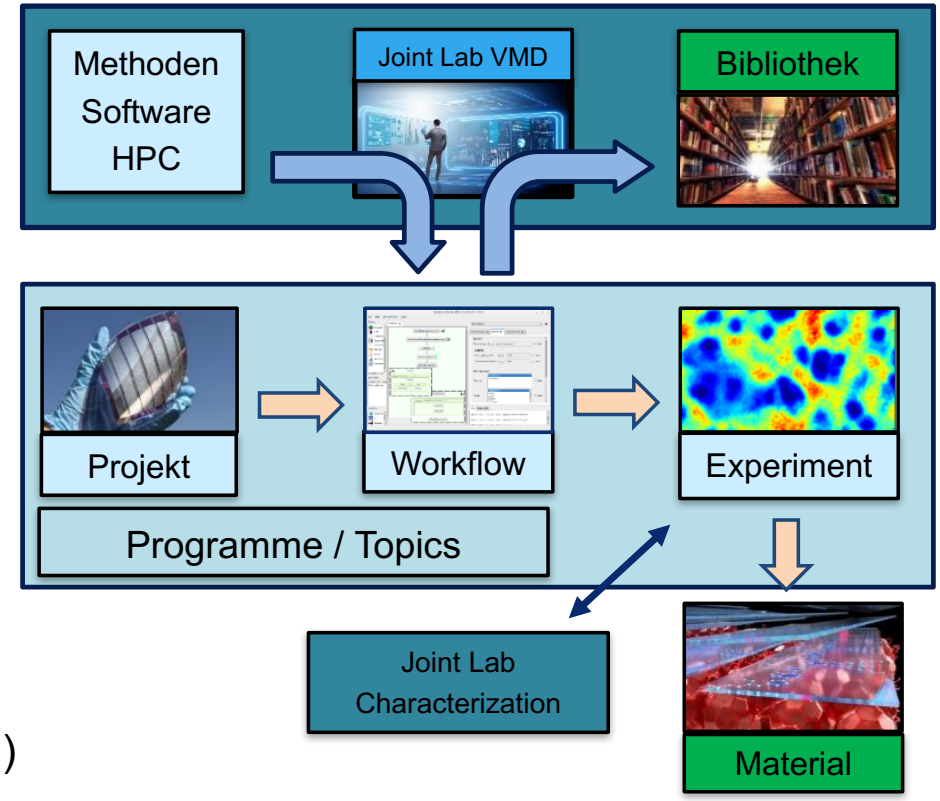
cp2k

AiiDA

Joint Lab Virtual Materials Design

Herangehensweise

- Helmholtz-Infrastruktur für die Digitalisierung von Materialien
- Entwicklung skalenüberbrückender und multiphysikalischer Methoden (P2/P3)
- HPC Code-Scaling, Performance Engineering und Weiterentwicklung für komplexe Rechnersysteme (Post-PetaScale) (P1)
- Effiziente Nutzung von künstlicher Intelligenz für materialspezifische Fragestellungen (P3/P1)
- Integration experimenteller Daten in den Modellbildungsprozesse (Topics P2/P3, JL Charakterisierung)



FUTURE PLANS

Scientific/Technical Challenges:

- Pushing the applicability and accuracy of DFT
- Code/Calculation stability
- Exascale computing

Workflows:

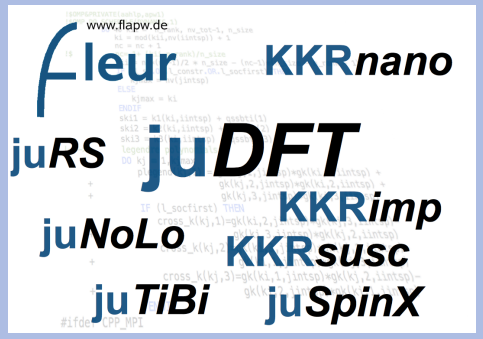
- Magnetic properties
- Model parameters
- Specific experimental accessible properties

Databases/Interfaces:

- Tailor made datasets for specific tasks
- Interfaces usable by non-experts
- Interfaces to Data Analytics Toolkits

SUMMARY

DFT to calculate materials properties



Example XPS spectra

- Workflow technology

- AiiDA, Python
- Creation of high quality DFT data

Jens Bröder

Stefan Blügel