Quantum-mechanics based materials design for novel quantum technologies: Activities and perspectives

Jürgen Spitaler
Materials Center Leoben Forschung GmbH

Shaping the future Quantum Technology Flagship – Workshop

Haus der Forschung/Wien, 18.01.2017
Materials Center Leoben Forschung GmbH

**Integrated Computational Material, Process and Product Engineering**

- **Mission:**
  - Fundamentals for *materials enabled innovations*
  - Hub for long-term strategic *partnerships science ↔ industry*
  - Hub for large *multidisciplinary projects*

- **Key figures:** 150 employees, 420 research partners, 15 Mio. € /year
Quantum-mechanics based materials design

Input
- Chemistry and crystal structure

Method
Solution of Schrödinger equation with levels of approximations:
- Density-functional theory (DFT) including fully relativistic treatment, spin-orbit coupling, on-site correlations, ...
- Many-body perturbation theory (hybrid functionals, GW, etc.)
- Time-dependent DFT
- Dynamical Mean-Field Theory

Output
- Total energies
- Electronic structure
- Phonons
- Magnetic properties
- Thermal behavior

Materials properties

Mechanical properties
• Plasticity: Stacking faults, screw dislocations
• Strength: Grain boundary embrittlement
• Elasticity

Thermal behavior
• Thermal expansion and phase stability
• Diffusion and segregation
• Defect formation

Functional properties
• Electronic properties: defect states, charge transfer
• Magnetism: magnetization, magnetic moment,
• Optical properties: dielectric function
• Ferroelectric behavior: polarization, piezoelectricity
Ab-initio methods for quantum technology

Examples

Search for nanostructures with thermally stable magnetization
- Systematic ab-initio study of metal dimers on defected graphene-based nanostructures
- Pt–Ir or Os–Ru dimers on defected graphene show giant magnetic anisotropy → promising systems

*Hu et Wu, Nano Letters 14 (2014), 1853*

Quantum anomalous and quantum spin Hall effect in doped kagome lattice Mott insulators
- New strategy for realizing these effects by hole and electron doping via chemical substitution.
- Ab-initio calculations show effect of chemical substitution on band structure and magnetic exchange

*Guterding, Jeschke & Valentí, Scientific Reports 6 (2016), 25988*

Control of the Metal-Organic Interfacial Electronic Structure
- Ab-initio based tuning of level alignment and substrate work function for organic molecules on noble metals
- guidelines for controlling charge-carrier injection in organic electronics

*Heimel, Romaner, Zojer, Bredas, Nano Letters 7 (2007), 932*
Status: Summary

- Quantum-mechanics simulation tools for materials highly developed

- Materials Center Leoben:
  - Development and application of quantum-mechanics based tools for materials science.
  - Fundamental research, method development and application
  - Mechanical, thermal, and electronic properties.

- Strong community in Austria for ab initio materials calculations:
  - 12 research groups (MCL, Uni Wien, TU Wien, Uni Graz, TU Graz)
  - World-leading codes (VASP, Wien2k)
  - 120,000 citations
Perspectives

Vision

*Integrated Computational Device Engineering for Novel Quantum Technologies*

Integration of
  - Experiment
  - Quantum theory
  - Ab-initio calculations
  - Model calculations

- Electronic states
- Magnetic properties (e.g. magnetic anisotropy energy)
- Electron-phonon coupling
- Materials properties of host systems (mechanical/thermal/electric behavior)
Thanks for your attention!