

Bachelor Projects:

- | | | |
|---|--|---|
| 1 | DFT Study of Topological Field Effect Transistor Germanene | 1 |
| 2 | Hall Effect: but Wait, Where is the Magnetic Field!!! | 2 |
| 3 | Spin transport in altermagnetic bilayers | 3 |
| 4 | Ab initio study of phonons of bulk layered non-centrosymmetric 4Ha-NbSe ₂ | 4 |
| 5 | w2dynamics: a (lively) dynamical mean field theory solver | 5 |
| 6 | Extending the Slave-Rotor Method to Multiorbital Interactions | 6 |

Bachelorarbeit
an Lehrstuhl
mit Zahl



An neuem
Lehrstuhl
"CQM"



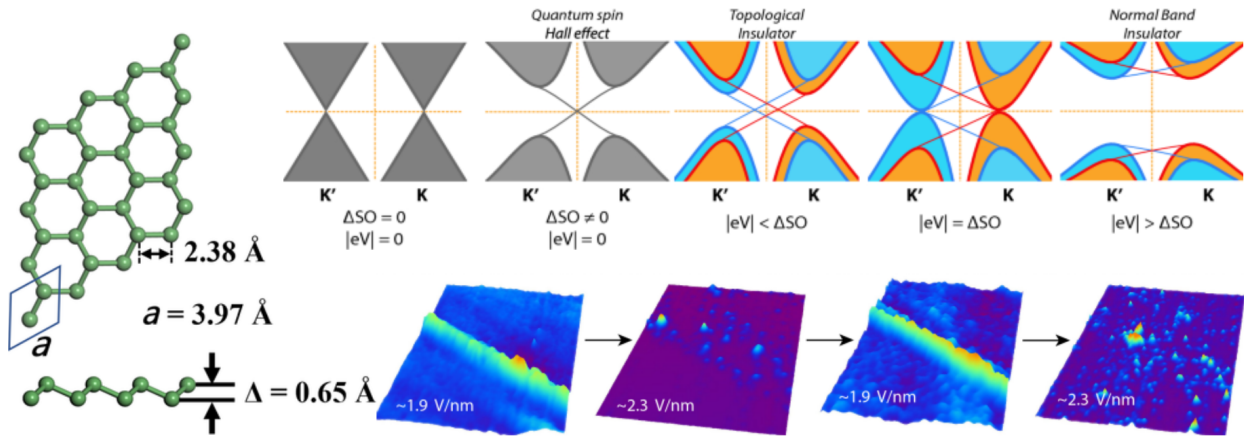
1 DFT Study of Topological Field Effect Transistor Germanene

Supervised by Stefan Enzner

Abstract

Two-dimensional (2D) materials with nontrivial topological properties have attracted attention for electronic device applications. One possible application is in **topological field-effect transistors**, which allow dissipation-free current flow through topologically protected edge states controlled by electric fields.

In this project, we investigate **germanene**, which is similar to graphene but has a buckled structure and stronger spin-orbit coupling. The material undergoes a phase transition from a topological to a trivial insulator, making it a promising candidate for a transistor. Using **density functional theory (DFT)** calculations, we study how an external electric field affects the electronic properties of germanene, such as its band structure and band gap. We will simulate 2D germanene as well as germanene slabs with edges to compare with experimental results and to assess the material's potential use in topological field-effect transistors.



Learning points

- Understand the fundamentals of **topological insulators** and the concept of **topologically protected edge states**.
- Learn to perform **DFT simulations** using computational tools (VASP or Quantum ESPRESSO) to study the electronic properties of materials.
- **Analyze data** with existing tools and own code snippets.
- Characterize band structures and identify signatures of **topological phase transitions**.
- **Interpret physical results**, linking band gap manipulation to real-world applications such as field-effect transistors.
- Develop **data visualization skills**, such as plotting band dispersions and possibly edge-state spectra.
- Gain experience in **scientific reporting, presenting**, literature comparison, and communicating complex phenomena clearly.

References

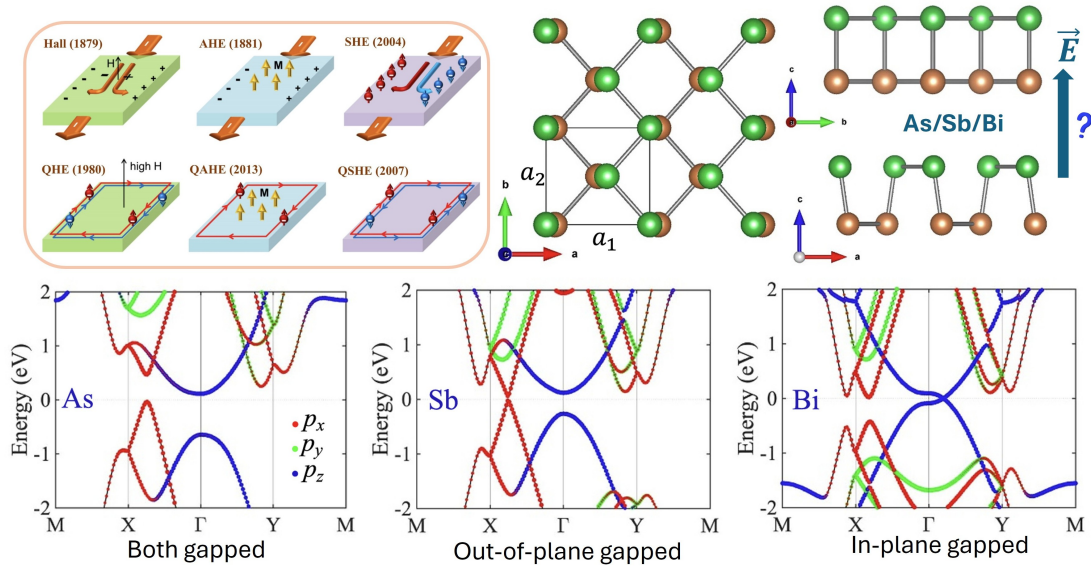
1. C. L. Kane and E. J. Mele, “ Z_2 topological order and the quantum spin Hall effect,” *Physical Review Letters*, vol. 95, no. 14, 146802, doi:10.1103/PhysRevLett.95.146802 (2005).
2. P. Bampoulis, “Quantum spin Hall states and topological phase transition in germanene,” *Phys. Rev. Lett.* 130, 196401, doi:10.1103/PhysRevLett.130.196401 (2023).

2 Hall Effect: but Wait, Where is the Magnetic Field!!!

Supervised by Dr. Arka Bandyopadhyay

Abstract

The Hall effect, discovered more than a century ago, revealed that electrons in solids do not always flow straight; they deflect in ways that encode the underlying quantum geometry of their wavefunctions. This insight laid the foundation for modern topological condensed-matter physics, where materials are classified using symmetry indicators associated with robust topological invariants and their protected edge states. Among the expanding family of Hall phenomena, the nonlinear Hall effect (NLHE) is particularly fascinating as it generates current that is quadratic in the applied electric field and it does not require any conventional magnetic field, magnetization, or in-general the time-reversal-symmetry breaking. This intriguing response originates not from the Berry curvature itself but from its first moment, the Berry curvature dipole (BCD), which captures the asymmetric distribution of Berry curvature in momentum space. Understanding and controlling the BCD has become a central focus in condensed-matter physics, driven both by fundamental interest and by its relevance to emerging technologies such as nonlinear photocurrent generation and terahertz detection. In this work, we uncover how orbital engineering satisfies the required symmetry conditions and enables NLHE in α -phase group-V monolayers—without the need for any magnetic field.



Learning points

- Develop practical skills in *DFT* (VASP, Quantum ESPRESSO), *Wannierization* (Wannier90), and topological analysis tools (WannierTools, WannierBerri).
- Understand how *orbital character*, *symmetry*, and *spin-orbit coupling* shape topological electronic structure.
- Learn to engineer and control the BCD and NLHE via electric fields and structural perturbations.
- Construct tight-binding models from DFT and connect them to measurable nonlinear transport signatures.
- Produce a coherent manuscript linking microscopic orbital physics to nonlinear quantum transport phenomena.

3-Month Timeline

Phase	Duration	Focus & Deliverables
Month 1: DFT	Weeks 1–4	Learn DFT workflows, reproduce α -As/Sb/Bi band structures, analyze orbital characters.
Month 2: Wannierization & TB Models	Weeks 5–8	Build minimal Hamiltonians, extract hopping/onsite terms, test electric-field perturbations, include SOC, compute Berry curvature, BCD and analyze NLHE.
Month 3: NLHE & Reporting	Weeks 9–12	write final report/manuscript.

References

1. Hasan, M. Zahid, and Charles L. Kane. "Colloquium: topological insulators." *Reviews of modern physics* 82.4 (2010): 3045-3067..
2. Sodemann, Inti, and Liang Fu. "Quantum nonlinear Hall effect induced by Berry curvature dipole in time-reversal invariant materials." *Physical review letters* 115.21 (2015): 216806.

3 Spin transport in altermagnetic bilayers

Supervised by Dr. Lorenzo Del Re

Abstract

Altermagnets (AM) are a newly discovered class of magnetic materials that display features resembling both more standard ferro and antiferromagnets (see Phys. Rev. X, 12.040501). The key distinction between a standard antiferromagnet and an altermagnet is **symmetry**: i.e. the two sublattices are related via a non trivial symmetry operation belonging the point group, i.e. a rotation or a mirror reflection. This peculiarity of these materials lift the so called Kramers degeneracy, i.e. spin-up and spin-down electronic bands are now split. This feature gives rise to a series of consequences such as non trivial transport properties of the spin making AM a promising platform for **spintronic** applications and quantum sensing.

Description of the project

The main topic of this project is the description of the ground state and dynamical excitations of bilayer spin systems whose geometry is set in a way to allow altermagnetic states. The student will learn theory methods for addressing Heisenberg spin-model, that read:

$$H = \sum_{ij} J_{ij}^{ab} \mathbf{S}_{i,a} \cdot \mathbf{S}_{j,b}, \quad (1)$$

where $\mathbf{S}_{i,a} = (S_{i,a}^x, S_{i,a}^y, S_{i,a}^z)$ are spin operators defining a SU(2)-algebra, i.e. $[S_{i,a}^\alpha, S_{j,b}^\beta] = i\epsilon_{\alpha\beta\gamma}\delta_{ij}\delta_{ab}S_{i,a}^\gamma$, i is the lattice index and $a = (t, b)$ indicates the top or bottom layer. J_{ij}^{ab} gives the structure of the spin interaction, intra-plane (when $a = b$) and inter-plane (when $a \neq b$). The application of such a project are related to the spin transport that this kind of bilayer systems can display, as for the example shown in Figure 1.

Mean-field analysis (1-4 week) : The student will familiarize with the Heisenberg Hamiltonian shown in Eq.1 and learn how to perform mean-field calculations to find what is the ground state of the system. This will give us insights about the magnetic phases as a function of different parameters defining J_{ij}^{ab} .

Spin-wave calculations (5-8 week) : After the ground state is found the student will learn how to add quantum-fluctuations to the mean-field solution using spin-wave formalism. This will allow us to have access to the magnon spectrum $\varepsilon_{\mathbf{k}s}$, where $\mathbf{k}$ is the crystalline momentum and s is the chirality of the magnon.

Spin-current calculations (9-12 week) : The student will become familiar with linear response theory and perform calculations of the spin-current J_ν^s , where $\nu = (x, y)$ are the cartesian directions, induced by a gradient temperature field quantified by the spin-conductivity tensor $\sigma_{\mu\nu}$ defined as $J_\nu^s = -\sigma_{\mu\nu}\nabla_\mu T$.

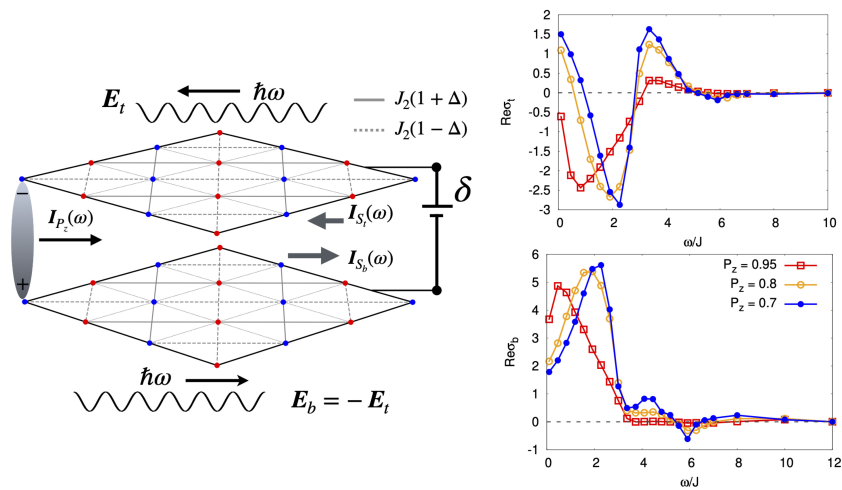


Figure 1: *Example of a bilayer system.* The gate voltage δ controls the layer polarization $P_z = n_t - n_b$. Blue and red sites represent the two spin sublattices. The inequivalent second-neighbor exchanges, $J_2(1 \pm \Delta)$, break translational symmetry and induce altermagnetic order. Counter-propagating electric fields couple to the layer dipole and, for $\Delta \neq 0$, generate a frequency-dependent spin current I_S . Adapted from arXiv:2508.06938, (2025), which resulted from a previous bachelor project.

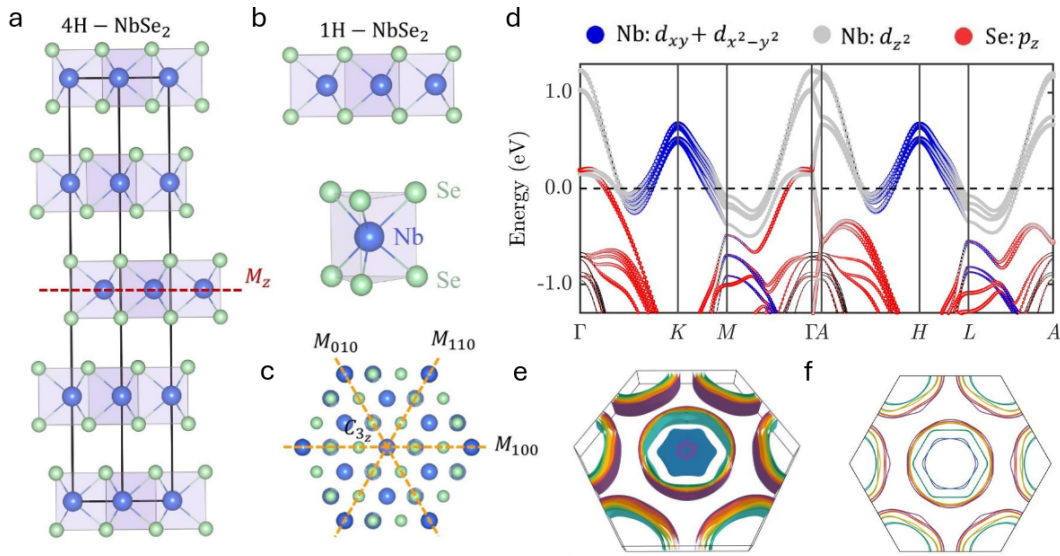
4 Ab initio study of phonons of bulk layered non-centrosymmetric 4H-NbSe₂

Supervised by Dr. Ludovica Zullo

Abstract

Transition metal dichalcogenides (TMDs: MX₂ where M is a transition metal and X is a chalcogen atom) are a class of layered materials, like graphene, in which layers may be exfoliated into single or few-layer sheets. Because of the distinct coordination in the monolayer, TMDs have various stacking sequences or polymorph in their bulk and multi-layer systems, which have a significant influence on their properties. Recently, a new TMD has been synthesized, the so-called acentric bulk superconducting polymorph, 4H-NbSe₂, which intrinsically breaks the inversion symmetry and supports valley-selective spin-polarized states and shows superconductivity at 6.2 K.

In this project, we investigate **4H-NbSe₂**, in comparison with its nearest and most famous 2H-NbSe₂ counterpart. We will simulate its band structure and phonon spectra to assess the material potential for superconductivity. Using **density functional theory (DFT)** calculations, we will study its band structure and by means of **density functional perturbation theory (DFPT)** we will calculate its vibrational properties.



Learning points

- Understand the fundamentals of **phonons**.
- Learn to perform **DFT and DFPT simulations** using computational tools (Quantum ESPRESSO) to study the electronic and vibrational properties of materials.
- **Analyze data** with existing tools and own code snippets.
- Characterize band structures and identify signatures of **charge density waves**.
- **Interpret physical results**, linking to superconductivity.
- Develop **data visualization skills**, such as plotting band dispersions and phonon spectra.
- Gain experience in **scientific reporting, presenting**, literature comparison, and communicating complex phenomena clearly.

References

1. L. Zullo, et. al., Phys. Rev. B 110, 075430 (2024).
2. D. Volavka et. al., arXiv:2501.08867 [cond-mat.supr-con] (2025).

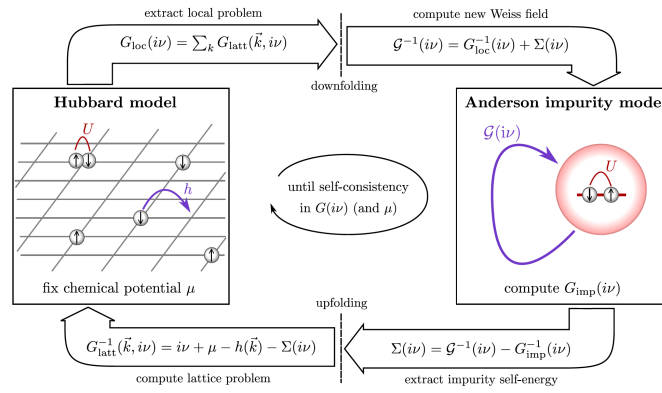
5 w2dynamics: a (lively) dynamical mean field theory solver

Supervised by Alena Lorenz

Abstract

Strongly correlated electron systems are an endless source of fascinating phenomena like Mott transitions or superconductivity. When dealing with such problems, it is quickly revealed that correlation between the electrons relates to an exponentially growing Fock space which therefore is limited by computational power/time to very few sites and orbitals. The single impurity Anderson model (SIAM) allows to treat such systems by singling out an orbital and treating it as an impurity embedded in the bulk of the material. A self-consistency condition arises whereby the bulk and the impurity (being the very same material) must exhibit the same behavior. The self-consistency loop is visualized in the figure below.

w2dynamics is a joint effort between JMU Würzburg and TU Wien. It uses continuous-time quantum Monte Carlo (CT-QMC) simulations to solve the SIAM. Although very powerful, we are long from done expanding this library. With new and exciting features implemented constantly, we need competent and motivated developers to keep on top of it all. This is where you come in!



3-Month Timeline

Phase	Duration	Focus & Deliverables
Month 1: DMFT	Weeks 1–4	Learn how w2dynamics is used. Get to play around with tutorials and past simulations. Get to know our local high-performance computer julia2.
Month 2: test new feature (e.g. mu-finder)	Weeks 5–8	Investigate the newest addition thoroughly with different Hamiltonians and interaction parameters.
Month 3: Complex calculation & Reporting	Weeks 9–12	Work on a more complex system with spin-orbit-coupling (SOC) and complex entries in the Hamiltonian.

Learning points

By the end of this project, you will:

- Understand the fundamentals of **quantum field theory** especially the **single Anderson impurity model**.
- Learn how to run the **DMFT solver w2dynamics**.
- Visualize and analyze simulation data in the a library of your choice.
- Get to know and love the **hdf5 file format**.
- Improved your problem solving skills.
- Know how to write a concise scientific report presenting all your hard work.

6 Extending the Slave-Rotor Method to Multiorbital Interactions

Supervised by Dr. Francesca Paoletti

Abstract

Strongly correlated electron systems are central to phenomena such as metal-insulator transitions, unconventional superconductivity, and complex magnetic ordering. In these materials, conventional one-electron approaches fail, making it difficult to obtain reliable theoretical descriptions. Among the theoretical tools developed to address strong correlations, the slave-rotor formalism provides an efficient method: it reformulates the interacting electron problem in terms of auxiliary fermionic (spinon) and bosonic (rotor) degrees of freedom and captures the Mott transition at moderate computational cost. However, the standard implementation of the slave-rotor technique remains limited to single-orbital Hubbard-type models, restricting its applicability to real materials where multiorbital effects do not play a fundamental role. This project aims to explore and develop an extension of the slave-rotor method to the (density-density) Kanamori interaction, opening the way for the study of Hund's physics within this framework.

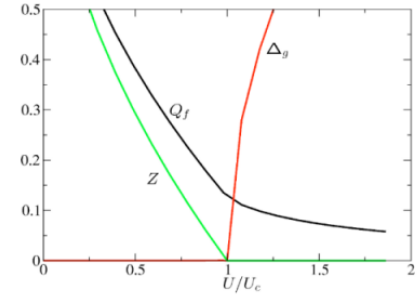
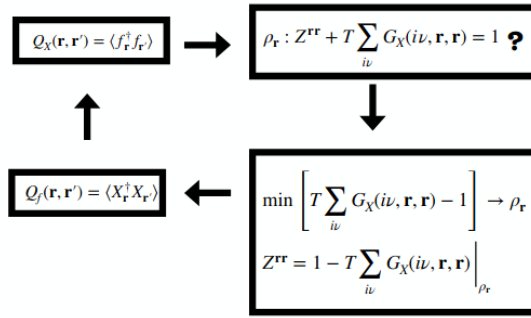


FIG. 9. (Color online) Plot of the quasiparticle weight Z , the effective mass renormalization $Q_f = m/m^*$, and the Mott gap Δ_M as a function of U/U_c across the Mott transition in the three-dimensional case.

3-Month Timeline

Phase	Duration	Focus & Deliverables
1. Become familiar with the physics of strong correlations	Weeks 1–2	Study the Hubbard and Kanamori models. Review the Mott transition and the beyond-mean-field techniques used to describe it.
2. Learn the slave-rotor method	Weeks 3–6	Read the seminal papers (Ref. 1) and understand existing limitations.
3. Carry out the calculations	Weeks 7–12	Attempt a concrete extension to two-orbital systems and report the results.

Depending on the interests and strengths of the student, the project may follow a more analytical route (deriving the "simplest" mean-field multiorbital rotor formulation) or a more numerical route (implementing the extended formalism within the group's existing slave-rotor code). Ideally, the chosen model would be the interacting Bernevig–Hughes–Zhang model, allowing the exploration of the interplay between topology and correlations.

Learning points

By the end of this project, you will acquire:

- A solid understanding of the Hubbard and Kanamori models and their relevance to strongly correlated materials, including the physics of Mott transitions.
- Familiarity with auxiliary-field methods, especially the slave-rotor formalism.
- Experience navigating the scientific literature.
- Improved problem-solving skills.
- (Optional) Hands-on experience implementing numerical codes for quantum many-body problems.
- The ability to write a concise scientific report presenting your results.

References

1. S. Florens, A. Georges, Phys. Rev. B 66, 165111 (2002) & Phys. Rev. B 70, 035114 (2004).
2. L. Crippa et al. Phys. Rev. B 104, 235117 (2021).