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| **Date** | **To do (both)** |
| 17-04 | * Time plan for project |
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| 24-04 | * Read both articles:   + Sødequist (2023) & Sødequist (2024) * Complete GPAW tutorial for spin spiral * Calculate propagation vector **Q** for MnI2 and VBr2 * Convergence checks for k-point sampling, cut-off energy for plane wave expansion etc. |
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| 01-05 | * SOC with PSO to calculate spin plane direction * Super cells without SOC to calculate energy and compare with GBT * Super cells with SOC to check error using PSO |
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| 08-05 | * First draft for report ready * Convergence checks for super cells… |
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| 15-05 | **Hand-in report!** |

Questions:

* Which functionals to consider? (LDA only, implementation issues)
* If Hubbard correction, what to use for U? (3-4 ev maybe, only for d-orbitals due to localization)
* How to check easy plane and Mermin-Wagner theorem?
* Time length of simulations? (HPC?)
* More materials? (NiI2)
* Spiral bandwidth?