

# Describing Quantum Phases of Matter and their Dynamics within Density Functional Theory and Time-Dependent Density Functional Theory

*Monday, 19 June 2017 09:30 (1h 15m)*

After an overview of the basic concepts of standard ground-state density functional theory (DFT) as well as time-dependent DFT (TDDFT), the description of quantum phases, such as magnetism and superconductivity will be addressed within this framework. The idea is to include the order parameter describing the respective phases explicitly [1,2] in the exchange-correlation functional of DFT/TDDFT. As a real-world example, the laser-induced demagnetization of ferromagnets [3] and the ultrafast magnetization transfer between sublattices of some Heusler compounds [4] will be calculated by real-time TDDFT. Furthermore, some thoughts will be presented on how to tackle topological phases of matter in a DFT/TDDFT framework [5], exemplified by the Berry phase [6] associated with the Beyond-Born-Oppenheimer description [7] of molecular motion.

[1] O.J. Wacker, R. Kuemmel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994).

[2] F.G. Eich, E.K.U. Gross, Phys. Rev. Lett. 111, 156401 (2013).

[3] K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, JCTC 11, 4870 (2015).

[4] P. Elliott, T. Müller, J. K. Dewhurst, S. Sharma, E. K. U. Gross, Scientific Repts 6, 38911(2016).

[5] R. Requist, E.K.U. Gross, Phys. Rev. Lett. 117, 193001 (2016).

[6] S.K. Min, A. Abedi, K.S. Kim, E.K.U. Gross, Phys. Rev. Lett. 113, 263004 (2014).

[7] A. Abedi, N.T. Maitra, E.K.U. Gross, Phys. Rev. Lett. 105, 123002 (2010).

**Presenter:** Prof. GROSS, E.K.U. (Max Planck Institute of Microstructure Physics)