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Report on the habilitation thesis entitled

Magnetization dynamics in solids studied by microscopic theory methods

submitted by

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to the Faculty of Mathematics and Physics, Charles University, Prague

After more than two decades of ongoing and still increasing research activities in spintronics that combines magnetism and electronics it is a well established field of solid state physics. The major reason for this is on the one hand side the many potential applications e.g. in storage and sensor technology based on spintronics. On the other hand, the new phenomena discovered in this field demand an adequate description for their full understanding and exploitation. Accordingly, solid state theory in particular when using methods based on density functional theory is indispensable to provide a detailed and realistic description of the various complex phenomena relevant for spintronics devices and their applications. The habilitation thesis of Dr. Carva reports on his many valuable contributions to the field that he made along this line during the last twelve years. Concerning this, emphasis was put on three subjects of central importance: *Magnetization dynamics in equilibrium*, *Magnetization dynamics induced by current* and *Ultrafast magnetization dynamics.*

The thesis starts with a short presentation of some well established basic concepts used to calculate exchange coupling parameters and the magnetic crystalline anisotropy energy and to account for finite temperature effects via the disordered local moment (DLM) model. Corresponding calculations allowed in particular to provide the necessary input for multi-scale studies making use of Monte Carlo techniques or done on the basis of the Landau-Lifshitz-Gilbert equation. The chapter *Magnetization dynamics in equilibrium* reports on a detailed study on the impact of defects on the magnetic properties of the anti-ferromagnet CuMnAs. The various types of lattice imperfections could be handled by means of the TB-LMTO-CPA (tight binding - linear muffin tin orbital - coherent potential approximation) electronic structure method that allows to account for the breaking of the Bloch symmetry due to defects and disorder. This powerful scheme was also used for an investigation of the Mn-doped topological insulator Bi_2Te_3. In this case, the CPA alloy theory permitted for finite Mn concentrations the calculation of the resistivity on the basis of Kubo's linear response formalism. The TB-LMTO-CPA provided also the technical basis for the studies on transport properties of layered systems presented in the chapter *Magnetization dynamics induced by current* that were formulated by means of the non-equilibrium Green function (NEGF) technique or the Landauer formalism, respectively. Formal developments allowed in this case detailed calculations of the so-called spin-mixing conductance as well as spin-transfer torque or torkance,

respectively, at interfaces of non-magnetic and magnetic materials. The last chapter entitled *Ultrafast magnetization dynamics* presents pioneering contributions of Dr. Carva and his colleagues to this most interesting topic that involves many different challenging aspects. The relaxation of a magnetic system after excitation with a strong laser pulse is to a large extent determined by the electron-phonon coupling. Detailed investigations on this so-called Elliott-Yafet mechanism could be performed on the basis of corresponding technical developments. The ab-initio electronic structure methods used allowed in particular to complement phenomenological approaches as for example the description of relaxation processes using the so-called three temperature model. Compared with work on transition metals, studies on rare earth systems have to account in addition for the complex electronic behavior of the f-electrons. To deal with this problem, it is assumed by Dr. Carva and his colleagues that a different magnetization dynamics is connected with the itinerant and localized states of an f-electron system. This concept could be applied successfully to various systems. A central issue of the phenomenon of ultrafast demagnetization is the dominating physical process behind it. Together with his colleagues, Dr. Carva could demonstrate the important role of super diffusive spin transport. The already mentioned linear response studies on the spin-transfer torque could be complemented by corresponding theoretical work on laser-induced spin-transfer torque. Strong laser pulses not only allow to destroy the magnetization but also to manipulate or switch it. Interesting corresponding theoretical work on this issue could be done again in collaboration. Most experimental studies on ultrafast magnetization dynamics make use of magneto-optical spectroscopies. For the proper interpretation of such experiments it is therefore of central importance to have an adequate accompanying theoretical description. Also to this issue several developments and contributions could be made by Dr. Carva and his colleagues.

Most of the work mentioned above was done together with various colleagues in a stimulating environment. In particular the work on magnetization dynamics, the central part of his thesis, was started when Dr. Carva was a post-doc with Prof. P. Oppeneer and Prof. O. Eriksson at Uppsala University. This fruitful collaboration was then continued until now. He could also collaborate on this topic with Prof. U. Nowak and Dr. D. Hinzke (University of Konstanz) who contributed with their well-known expertise in statistical methods. In addition to the common work with colleagues from theory, Dr. Carva could complement experimental work on phonons ultrafast demagnetization using magneto-optical techniques done by Prof. H. Dürr (SLAC, Menlo Park; now Uppsala University) and Dr. P. Grychtol and Dr. E. Turgut (University of Colorado and NIST), respectively. These ongoing fruitful cooperative work reflect the interest of other scientists to benefit from Dr. Carva's expertise as well as his ability to collaborate with others.

The interesting results of the research work of Dr. Carva was documented in more than sixty publications in journals of high international rank, with fifteen of them with him as first author. In this context one has to mention in particular the contributions to the most prestigious journals *Physical Review Letters* (four), *Nature Communications* (three) and *Nature Physics* (two). Furthermore, one should mention his contribution *Laser-Induced Ultrafast Magnetic Phenomena* - together with Pavel Baláž and Ilie Radu - to the 2017 issue of the Handbook of Magnetic Materials. All his published works make him well visible in the scientific community. Their rank is in particular reflected in the number of citations (more than 1300) or citations per publication (about 22), respectively, and the h-index of 18, that is fully adequate for

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his age and state of career. May be, the scientific independence of Dr. Carva could be underlined even more by adding some papers to his publication list with him as only author.

Dr. Carva obviously has already quite some experience in teaching giving regularly seminars and lectures in Solid State and Computational Physics and related fields. Furthermore, he already supervised several bachelor, diploma and Ph.D. students working on various topics of great current interest in spintronics.

In summary, one can say that the thesis, that is of high international standard, reflects the very productive, continuous and successful activities of Dr. Carva over the years in a rapidly developing and competitive field of solid state theory. As he could demonstrate, he was able to apply successfully a broad range of techniques and methods to many different aspects of magnetism that are relevant in particular for spintronics. As much of the work was done in collaboration with other colleagues, Dr. Carva should perhaps underline more his scientific independence in the future by corresponding publications. However, this should be seen as a minor comment. Accordingly, I don't hesitate to strongly recommend acceptance of the presented thesis in its present version.

Prof. Dr. Hubert Ebert

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