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## Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

Tuesday, 23 Mar. 2021, 9:00 s.t., UDE, Zoom



**Prof. Dr. Samir Lounis**

**Functional Nanoscale Structure Probe  
and Simulation Laboratory,  
Forschungszentrum Jülich**

Zoom information:

Meeting-ID: 865 9273 0403

Kenncode: 001347

### Complex magnetism at the nanoscale: from skyrmions down to single adatoms

#### Abstract:

Functional magnetic materials are key elements in many present-day technologies, and their physics spans many orders of magnitude in length and timescales. This poses great challenges for computational materials modelling. In this talk, I will present some highlights of our work combining the development of novel theoretical approaches and cutting edge methodologies that harness modern supercomputing resources in order to answer some of those challenges. I will focus on two important aspects: magnetic fluctuations and defects, which determine several physical properties of a material and the viability of a device. Spin fluctuations, being thermal or quantum, are expected to be enhanced when reducing the dimensionality of a material or when competing magnetic interactions are present. They lead to the temperature dependence of the magnetic anisotropy energy, which sets an upper limit to the coercive field of permanent magnets, and are directly exploited in magnetocaloric cooling, as they control the relative stability of different and possibly competing magnetic phases. I will address quantum magnetic fluctuations in atomic-scale magnets and their implication in designing their hysteresis while reshaping a whole set of magnetic interactions [1,2,3]. Then I will demonstrate how the latter are renormalized by thermal fluctuations, which allows us to solve the magnetic puzzle of B20-MnGe characterized by a three-dimensional spin-texture, for which we recover the magnetic phase diagram when we account for higher order interactions [4,5]. Finally, I will show that the energy landscape of topological spin-swirling spin-textures, so-called magnetic skyrmions, obey a universal behavior when interacting with transition metal defects [6]. The latter can be very useful by enabling either optical or all-electrical detection mechanisms [7].

[1] Ibanez-Azpiroz, dos Santos Dias, Blügel, Lounis, Nanoletters 16, 4305 (2016)

[2] Bouaziz, Ibanez-Azpiroz, Guimaraes, Lounis, Phys. Rev. Res. 2, 043357 (2020)

[3] Bouaziz, Guimaraes, Lounis, Nat. Commun. 11, 6112 (2020)

[4] Mendive-Tapia, dos Santos Dias, Grytsiuk, Staunton, Blügel, Lounis, Phys. Rev. B 103, 024410 (2021)

[5] Bornemann, Grytsiuk, Baumeister, dos Santos Dias, Zeller, Lounis, Blügel, JPCM 31, 485801 (2019)

[6] Fernandes, Bouaziz, Blügel, Lounis, Nature Communications 9, 1 (2018)

[7] Fernandes, Bouhassoune, Lounis, Nature Communications 11, 1602 (2020)

#### About the speaker:

Samir Lounis is Professor at the University of Duisburg-Essen since November 2020 and head of Funsilab at Forschungszentrum Jülich since January 2011. From 2015 till 2020 he was Junior Professor at the RWTH-Aachen University. His research synergizes theoretical condensed matter physics and computational materials modelling, with a special focus on magnetic properties of systems of all dimensionalities, going from adatoms and clusters on surfaces to magnetic thin films and bulk materials, and large-scale structures such as magnetic skyrmions. After a PhD in Physics (2007) defended at the RWTH-Aachen University under the supervision of Stefan Blügel and Peter H. Dederichs, he was postdoc with Doug L. Mills at UC Irvine with a Feodor-Lynen Fellowship (2009-2010). His group benefitted from strong funding of the Helmholtz Association of Research Centres (2011-2016) and of the European Research Council (Consolidator grant – Dynasore, 2016-2021).

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