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EUSpec - Modern tools for spectroscopy on advanced materials: a European modelling platform

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The study of materials is of central significance for progress in science and technology. At present the focus is on materials with reduced dimensions such as nano-structures or molecule based systems. These materials offer new tunable properties. In order use them in devices a deep understanding of the properties of the materials on the atomic scale is a prerequisite. Non-destructive spectroscopies are a fundamental tool of analysis at the nanoscopic level, allowing to probe matter and its constituents with an atomic resolution, and to monitor their time evolution down to the femtosecond range, transforming them into unique methods to trace chemical reactions. However, in order to make use of the continuously increasing resolution in space, energy, momentum, spin and time, complementary theoretical support is indispensable. This is where new EU-funded COST action EUSpec gets in. This COST action brings together the expertise of experts working in the science of advanced materials in order to build a coherent theory and computing platform with a new common data format to model sophisticated spectroscopy experiments performed at advanced radiation sources as well as at academic and industrial research laboratories. The goal is to strengthen the communication between between theoreticians and experimentalists because on the one hand new types of experiments are important benchmarks for the status of theory and often require or trigger new formal theoretical and corresponding code developments. On the other hand, experimental groups are not always aware of the available tools and program packages provided to them by the colleagues from theory to analyze and interpret the experimental findings. EUSpec will lead to a large-scale network in order to give a strong impetus to the spectroscopy research and to give Europe a decisive lead. It will establish a platform that goes far beyond the applicability of the actual individual computational codes in order to address the relevant questions and problems for many more materials and spectroscopies. In line with these ambitious goals, EUSpec will be presented to initiate strong interactions between theory and experiment in the future.

References

http://www.euspec.eu/

Primary author: Dr SUBIAS-PERUGA, Gloria (ICMA, CSIC-Universidad de Zaragoza)

Co-authors: Dr SEBILLEAU, Didier (Université de Rennes-1); Prof. HERPER, Heike (Uppsala University); Prof. EBERT, Hubert (University of Munich)

Presenter: Dr SUBIAS-PERUGA, Gloria (ICMA, CSIC-Universidad de Zaragoza)

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