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Theory of novel spectroscopic techniques: Probing spin, charge and orbital physics

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Abstract. Transition metal compounds show many fascinating properties that can be exploited in sensors, next generation electronics, and in catalysis for chemical reactions. Bulk materials exhibit high-temperature superconductivity, colossal magneto resistance, metal-insulator transitions, and many more exotic properties. Nanoclusters, surfaces, and interfaces provide us with the opportunity to combine and tune these fascinating properties, in obtaining novel functionalities. This is also the case when transition-metal ions are introduced in an organic molecule, as beautifully realized in nature with the active role Mn atoms have in the fundamental process of photosynthesis. The astonishing electronic and magnetic phenomena stem from the delicate interplay of the spin, charge, and orbital degrees of freedom associated with the open-shell transition metal ions. Their understanding and exploitation embody the central scientific questions challenging the field of condensed matter physics. The development of novel computational approaches, as well as the deeper theoretical understanding of modern electron spectroscopies, has recently enabled us to disentangle the role of these different low-energy degrees of freedom. In this talk I will illustrate — with a few selected examples — how theory is contributing to the refinement of modern spectroscopic techniques and to the furthering of our microscopic understanding of the spin, charge, and orbital interplay in complex materials.