New Quantum-Chemical Methods and New Applications: NMR/EPR Parameters, Local Hybrid Functionals, and more.

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In my lecture I will give an overview on some of the recent activities in our group, encompassing a wide range of methodological developments and applications. In the field of magnetic-resonance parameters, I will focus on spin-orbit effects on NMR shifts, both for closed-shell systems,[1] and for paramagnetic systems. The latter case reaches from the long-range pseudo-contact shifts in an entire metalloprotein domain[2] to a full treatment of contact, pseudo-contact, and orbital shifts in extended solids (with applications to lithium-ion battery cathode materials[3] or even MOFs[4]). Time permitting, I will also mention briefly some recent advanced spin-projection procedures for EPR and INS spectra of single-molecule magnets.[5] In the second part of my talk I will focus on our extensive development and first applications of local hybrid functionals with position-dependent exact-exchange admixture.[6] This includes the appreciable potential of local hybrids for excited states[7] and for NMR/EPR parameters,[8] as well as validation and application to the question of localization/delocalization in mixed-valence systems.[9]

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