From the development of theoretical models to applications in Chemistry

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The need to understand the microscopic mechanism underlying complex chemical phenomena is a strong driving force for the development of new theoretical models. In recent years a further boost has come from models that can provide chemical and physical properties with accuracy comparable to that obtained from experiments, if not, in some cases, better. It is no a mere coincidence, then, that these theoretical models have left the purely academic level and entered not only into industrial R&D but also into legislation (see, for example, the European REACH regulation). This also applies to models based on the so-called Density Functional Theory (DFT), which are widely used in Chemistry and Physics to model the electronic structure of matter (and its properties).
Nevertheless, the perfect computational approach does not exists and there is still room for improvement in both accuracy and area of application. Indeed, better performing DFT models are systematically proposed, in order to address the known drawbacks and further expand the domain of applicability.
In this talk, we describe our approach to developing new DFT models that, starting from purely theoretical constraints, allows to define new nonempirical methods whose performances are comparable to that obtained from models tuned on specific properties. The discussion of selected applications in Chemistry not only shows the wide domain of applicability of our nonempirical models, but also emphasizes how increasing the number of theoretical constraints induces improved accuracy on chemical and physical properties.