Quantum chemistry solutions for molecules with heavy atoms in realistic environments. Description for the general public

Małgorzata Olejniczak

Almost every day we hear about innovations in functional materials or drugs design. The search for new materials of desired functionalities is on one hand a necessity (e.g. renewable energy sources) and on the other – a way to improve conditions of life of modern societies (e.g. responsive materials used in medicine). Many of such materials contain heavy atoms – of elements from the bottom of the periodic table. The heaviest – lanthanides and actinides – are radioactive and used in nuclear medicine or as energy sources (nuclear fuel), slightly lighter are used in catalysis (e.g. platinum, silver) or as topological insulators (bismuth, antimony) important for research on superconductors and considered for building quantum computers. Another important issue is high toxicity of heavy elements for living organisms (they are considered as one of responsible factors in neurodegenerative conditions such as Parkinson's or Alzheimer's diseases), therefore their monitoring in environment and living cells is also crucial.

Efficient design of solutions for the sustainable future depends on the profound understanding of the relationship between structure, function and properties of atoms and molecules in their real environments, e.g. in condensed phases, on interfaces, in structures complex molecular assemblies (nanotubes, molecular layers, crystals). Insight into the processes in the atomic and molecular scale, the change in molecular properties caused for instance by the interactions with other molecules or with electromagnetic field and relating them to the macroscale is not only important to design and improve functional materials, but also allows to answer some basic research questions in life sciences.

The main research techniques unravelling the atomic world are spectroscopy and (related to it) quantum chemistry. Spectroscopic techniques measure the response of the matter to e.g. perturbing electromagnetic field. This response is inherently connected to the electronic structure of the matter, which is the central subject of studies in quantum chemistry. The development of new methods in quantum chemistry allowing for the determination of electronic structure and molecular properties (related to observables in spectroscopy) of molecules with heavy atoms in realistic environments constitutes the main objective of this project. Calculations with such methods will not only allow to interpret molecular spectra, but also are very often the only source of information on the electronic structure of molecular systems for which experiments cannot be performed or are too expensive. The most important equations in quantum chemistry cannot be solved analytically, therefore the main work of a quantum chemist is to design approximate computational models which are accurate enough for the property and system of interest. Practical use of such methods is computationally very expensive, therefore one of the major challenges of quantum chemistry is compromising the accuracy and cost of calculations. The more complex molecular system is studied, the more difficult this compromise is to reach. This is the case for molecular systems with heavy atoms. Their presence requires a good descriptions of the so-called relativistic effects, related to the increased mass of electrons in the proximity of heavy nucleus and to magnetic interactions. These effects can only be studied by theoretical methods (as our world is inherently relativistic) and their most interesting manifestation is for instance the yellow color of gold or the liquid state of mercury in the room temperature. Additional difficulty in such calculations is due to the presence of an environment of the molecule of interest, which can significantly affect its geometry, electronic structure and molecular properties. An interesting theoretical approach is to use embedding methods, in which a molecule is considered as embedded in an environment of other molecules represented by an effective potential. An exact prescription is given by the frozen density embedding (FDE) method, which constitutes the main framework for developments in this project. FDE will be extended to relativistic formalism, what will allow to perform calculations with relativistic and environmental effects accounted for from the start and to understand properties of molecules with heavy elements in various (also complex) environments. This project contributes to the basic research in life sciences, however as the proposed methodology can be considered as a bridge between atomic and macroscopic scales, it has also a high application potential. In particular, the systems for which the calculations will be performed in this project can be used as pharmaceuticals, magnetic molecular materials and chemical sensors.