

## Research Interests of Dr. Laura Gagliardi

My research in future years will be focused both on applications and method development in computational chemistry. One of my major fields of research is quantum inorganic chemistry. This area comprises transition metal chemistry, lanthanide and actinide chemistry with the aim of understanding properties of existing species and predicting the existence of new species. I plan to continue this research and deepen aspects that I have not considered so far.

I would like to undertake research in the following general areas:

- Prediction of chemical species as new materials
- Heavy element chemistry in gas phase and in solution
- Development of new computational tools for heavy element chemistry
- Study of evaporation and condensation phenomena in early minerals

I intend to investigate new species containing metals which could be considered the building blocks for nanomaterials. Gold chemistry for example has unexplored properties. Gold is a versatile element and new metal-golden clusters are highly likely to be invented. The mixed metal-polyhydrogen compounds will also be investigated systematically in order to design improved systems for the hydrogen storage problem. A possible collaboration on some catalysis problems involving transition metals and lanthanides has been recently discussed with Professor Bart Hessen, Groningen University.

I plan to continue to work in actinide chemistry and study systems like the uranium diatomic molecule  $U_2$  and other diactinide compounds. These systems may open new frontiers in the area of catalysis and synthetic chemistry and are challenging from a computational point of view. Preliminary results indicate that the uranium molecule  $U_2$  has six valence unpaired electrons

which may give rise to new chemical bondings. New systems like  $\text{NU}_2\text{N}$  or  $\text{Cl}_3\text{U}_2\text{Cl}_3$ , in analogy to the well known  $\text{Re}_2\text{Cl}_8^{2-}$  species could well exist and are worth exploring.

Heavy metal chemistry in solution will also be addressed. Over the years I have developed some experience in studying such systems in solution by treating at the quantum level actinide complexes and modeling the solvent environment by a continuum with a reaction field Hamiltonian. With this approach uranyl and neptunyl complexes in water have been investigated. However, the investigation of the solvation of such complexes using a continuum model and some explicit solvent molecules is only a partial way of treating the problem.

This topic of research will thus involve both new applications and method development. A different approach, a combination of quantum chemistry and statistical mechanics needs to be utilized. The quantum chemical side will be based on accurate calculations of molecular properties in ground and excited states of molecules in solution. The solvent effects will be taken into account dynamically. The method could be based on a non empirical model potential model, like for example the NEMO model, which has been developed by Professor Gunnar Karlström and his collaborators in Lund. The approach has hitherto mainly been used for weak interactions between neutral molecules. I plan to bring an innovative contribution to the field by extending the scheme to the treatment of strongly interacting multi-charged ions with solvent molecules. The conventional approach of using empirical or semi-empirical potentials is not desirable for this type of systems, because very little experimental information is known and even if one could generate an empirical potential for one of them, it would not be easy transferable to others. I have initiated research in this field, but major work still remains to be done and I intend to develop such research in the future years.

I would also like to explore new frontiers in density functional theory in order to study large systems containing heavy elements. Multiconfigurational methods like the CASSCF/CASPT2 approach do an excellent job on heavy element systems, but the dimensions of the calculations become easily prohibitive. Current DFT codes including relativistic effects, using Gaussian basis sets, often suffer from convergence problems and problems related to the single-configurational

nature of the DFT approach. New ways of doing DFT need to be explored.

I plan to extend my interests towards a more 'macroscopic' scale. This direction is already evident from the necessity of addressing the problem of heavy element ions in solution with a combined quantum mechanical and classical mechanical approach. In more general terms, I would like to investigate problems related for example to the evaporation/condensation of early minerals, a topic of much interest in the geochemistry and geophysics community. This research would involve in a first stage the use of quantum chemical methods at the molecular level, but it will also require the use and, eventually, the development of new methodologies to study periodic systems.

Over the past years I have also developed an expertise in studying spectroscopy of organic molecules. I believe that this area is also important for applications of quantum chemistry and I plan to continue this research and extend it to the study of photochemical reactions in the gas and condensed phase.

I have always benefited from the collaboration with various scientists in my career and I have enjoyed it both from the professional and personal point of view. I intend to continue to do so also in the future because I think that the development of new ideas and research strategies are greatly enhanced through the interaction with other experts in the field.

It would be easy to involve future students in the various areas of my research. Master students could be easily take part in short term application projects, while PhD students could also contribute to the method development research. In the past years I have given courses on quantum mechanics, spectroscopy and physical chemistry to undergraduates and I have been exercise leader at the European Summer School in Quantum Chemistry. I consider teaching a fundamental part of the academic job and I am delighted to contribute to the teaching responsibilities of the Department.