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Computational modelling of functional materials and chemical reactivity using molecular dynamics, DFT and wave-function-based approaches

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Quantum chemical methods, in particular, those based on density functional theory (DFT), can be successfully used to achieve a mechanistic understanding of reactivity at the microscopic level, which is required to optimise functional materials (such as catalysts, electrocatalysts, semiconductors, optoelectronic materials) with respect to their target properties.

The presentation will highlight the various research topics and achievements of the research programme led by L. Moskaleva at UFS. Our research applies the tools of computational chemistry to study phenomena such as gas-phase reactions, reactions in solution and at solid surfaces.

We apply DFT methods, wave-function based methods, ab initio molecular dynamics (AIMD) simulations, and microkinetic modelling to study material properties and complex reaction mechanisms, either in the gas phase, or on various solid transition-metal catalysts, including rare earth oxides and coinage metals, in particular on Au-Ag alloys. Our research efforts have been largely focused on nanoporous gold (np-Au), a novel catalyst proposed for environmentally friendly applications but also an interesting material from the point of view of fundamental research on gold. Since the discovery of the catalytic activity of gold at the nanoscale, as opposed to the very inert bulk Au, there has been an ongoing debate in the scientific community, as to whether gold on its own (without any support material) can be catalytically active. Our research has contributed to this scientific debate and related questions about the interplay between the topology, composition, and catalytic properties of alloyed nanostructures.

We also work on the topics related to chemical kinetics of hydrocarbon combustion and on functional materials, such as luminescent organometallic complexes. In collaboration with experimentalists, we have computationally characterised a series of luminescent binuclear Au-Au complexes with N-substituted bis(diphenylphosphino)amine ligands. Our time-dependent density functional theory (TDDFT) calculations provided valuable insights into the interpretation of the photophysical properties of the complexes, highlighting the phosphorescent nature of the emission and explaining the differences in emission wavelengths observed between complexes with different counterions.

We are grateful to the CHPC for providing state-of-the-art computing facilities that allow us to use computational chemistry software and perform sophisticated calculations of molecular and crystalline systems.

Student or Postdoc?

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Workshop Duration

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