# LUMPAC LUMinescence PACkage: New methods and implementations

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## INTRODUCTION

The systems containing lanthanide have been widely studied due to their several applications such as in luminescent sensor, optical fibers, biologic markers, and luminescent devices. The search for new lanthanide systems can be carry out only by using theoretical methods. Due to lack of a computational tool with these methods implemented, the LUMPAC[1] (LUMinescence PACkage) software was developed and is available free of charge at http://www.lumpac.pro.br.

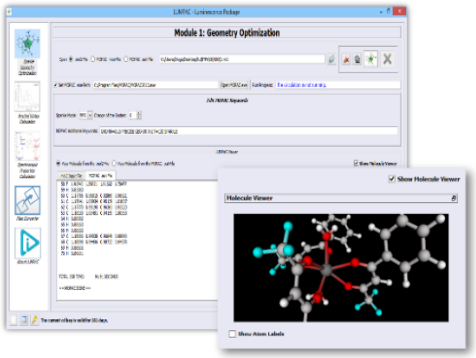


**Figure 1**. LUMPAC software.

LUMPAC is structured in modules. The first and second one are integrated to the MOPAC and ORCA programs, respectively, enabling the geometry optimization of the system and the excited states calculations of the ligand part. The third module calculates the luminescence properties, such as experimental and theoretical intensity parameters ($\Omega_\lambda$), energy transfer rates, and theoretical emission quantum yield. The fourth module is a file converter. In the first version of LUMPAC were just implemented some of the main methods commonly applied to study luminescence properties of lanthanide systems. This work aims to present the new methods and implementations that were added to the second version of LUMPAC.

## RESULTS AND DISCUSSION

Currently, we are reparameterizing the INDO/S-CIS semiempirical method, which is implemented into ORCA. At the end, we hope to obtain a method with similar accuracy compared to TD-DFT method for the excited states calculations of systems containing lanthanide. A new submodule that enables the phenomenological calculation of the Stark levels was added to the third module. From this calculation, the ligand field parameters ($B_{kq}$) are obtained. In the submodule regarding the calculation of energy transfer rates, we implemented the model developed by Malta and coworkers to calculate the energy transfer in systems with charge transfer band[2]. Furthermore, the model improved by Malta to calculate the energy transfer rates between two lanthanide ions[3] was also implemented into this new version of LUMPAC.

## CONCLUSIONS

All these new implementations become LUMPAC a tool ever more useful for that research groups interested in understanding the photophysical properties of systems containing lanthanide ions. In a little more than one year, we already distributed more than 100 licenses throughout the world.

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