COMPLEXSIM

Computational simulation of complex reaction mixtures

Timeline | 09/2024 to 08/2027

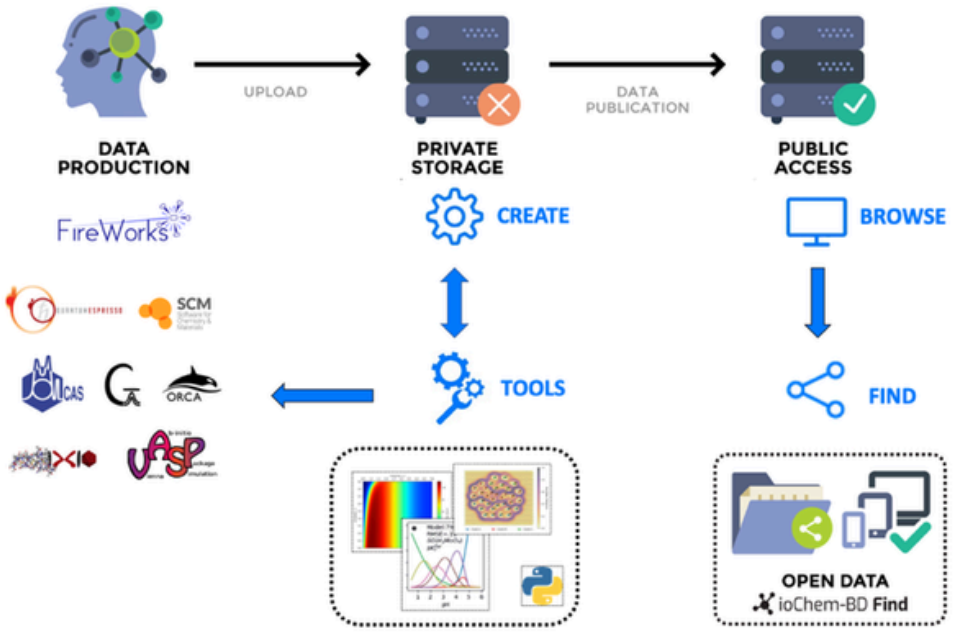
ICIQ People | Carles Bo Research Group

Budget | 150.000 €

Call | Proyectos I+D
Generación Conocimiento 2023

SUMMARY

The COMPLEXSIM project aims to develop and apply new computational methods for studying complex reactive mixtures of metal oxide species in solution, such as those formed in the field of polyoxometalates. Based on our recently developed method, phase speciation diagrams (concentration vs. pH) of various heteropolyoxometalates, such as Keggin, Anderson, and Wells-Dawson anions, will be determined directly from DFT methods. The obtained reaction networks will be used to construct massive micro-kinetic models, allowing for a direct comparison with recent experimental results suggesting autocatalytic mechanisms. In addition to addressing fundamental issues in polyoxometalate chemistry, this project will investigate the effect of relevant parameters such as solvent, temperature, and pressure on phase speciation diagrams. There is still a complete lack of understanding of how organic solvents direct regioselectivity in the synthesis of POMs, or what happens inside reactors under hydrothermal conditions. On the other hand, this project aims to develop new methods for treating redox reactions in systems with metals in multiple oxidation states. Additionally, ML/AI techniques will be explored to develop atomic potentials to accelerate the discovery of new materials. This part of the project involves creating databases that will be reused both to train ML/AI methods and to develop a user interface tool within the ioChem-BD platform.



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