CompChem-4.0

Computational Chemistry 4.0 for a Sustainable Development

Timeline | 09/2021 to 08/2024

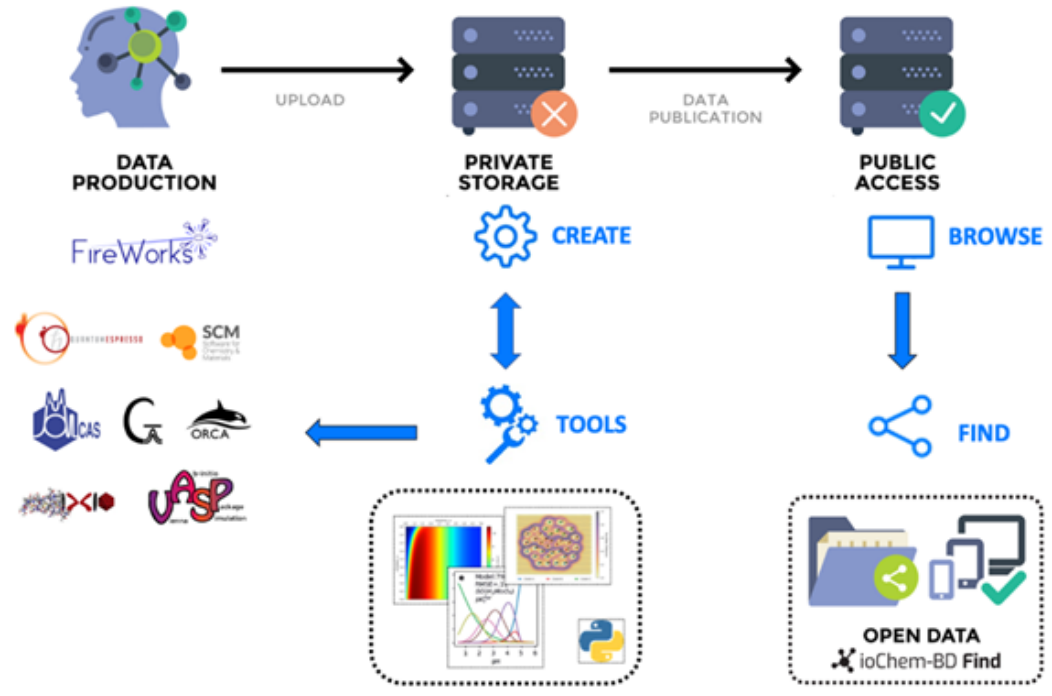
Budget | 121,000 €

ICIQ People | Carles Bo Research Group

Call | Proyectos I+D - Retos Investigación 2020

SUMMARY

This project is aimed at applying modern computational chemistry methods to solve problems in the fields of catalysis and nanoscience, some of those called emerging chemical technologies that show great promise for alleviating important societal problems and for a sustainable development. We expect to provide rules to discover new process to convert CO_2 into useful chemicals, to improve C-C oxidation reactions, and to discover new catalysts for the H_2 evolution reaction. We also expect to make significant contributions to the understanding of the chemistry of metal oxides and to predict properties of new species. In most cases, given that a good part of the investigation is planned in direct collaboration with experimental groups that are leaders in each field, it is expected that the synergies between experiment and theory will promote breakthrough advances on both sides. Moreover, aligned with the Chemistry 4.0 principles, digitization and open-data movement, we aim at developing unique software tools and databases for accelerating catalysts design.



Reference: PID2020-112806RB-100