Data4Mat

Linked chemical databases to boost materials discovery

Timeline | 12/20222 to 11/2024

Budget | 172.500 €

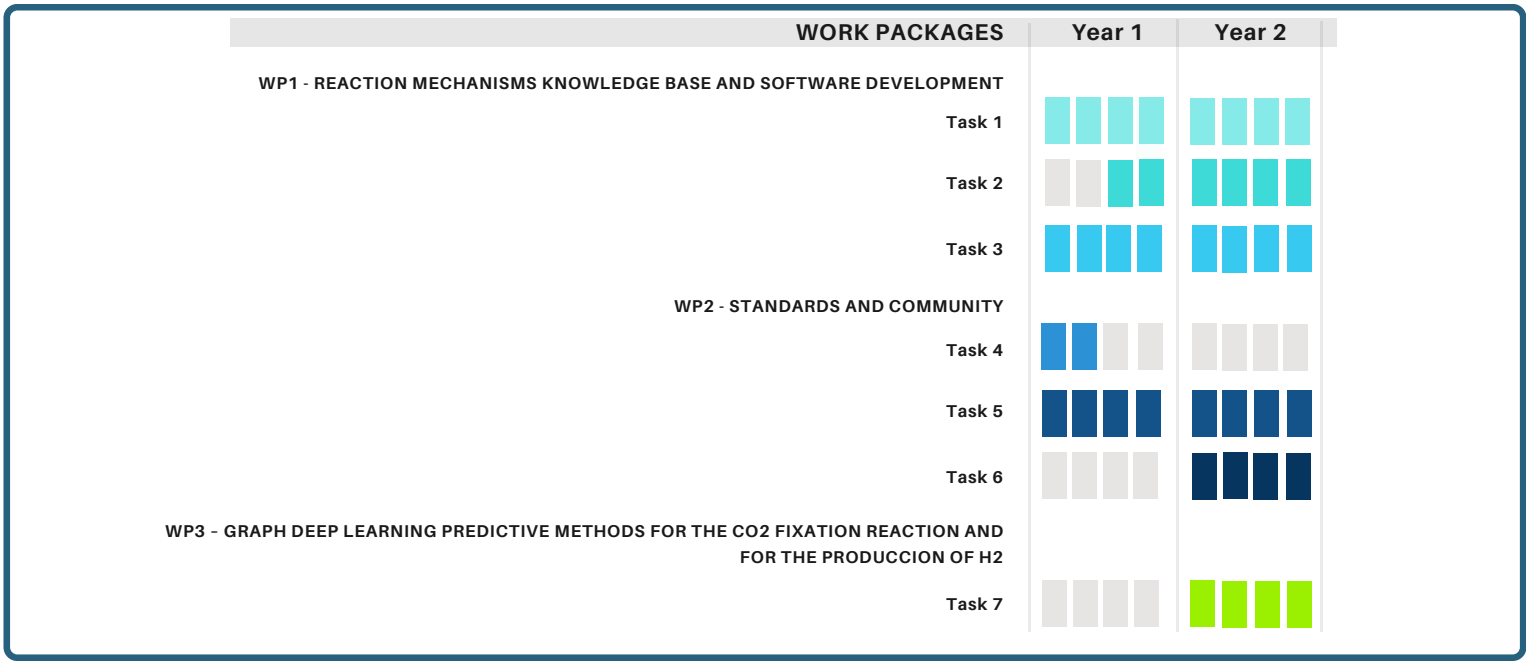
ICIQ People | Carles Bo Research Group

Call | Proyectos estratégicos orientados a la Transición Ecológica y a la Transición Digital 2021

SUMMARY

Data4Mat will boost the digital discovering of new catalysts to help solving crucial societal challenges such are the climate change and the quest for alternative energies sources by applying modern computational chemistry methods and advanced data treatment. Fixing CO2 to create value-added chemicals as are organic carbonates and/or polycarbonates, and finding catalytic materials to form hydrogen efficiently are the two main targets of the project. To do so we propose the creation of what we call the Reaction Mechanisms Knowledge Base, that is a new kind of well-structured database that will allow representing all the chemical knowledge and properties about catalytic processes in a comprehensive and machine-readable way. Digitalizing chemical and catalysis data, based on ontologies, will allow inferring new properties thanks to the straightforward connection to other databases, to develop predictive graph deep-learning methods, and to accelerate catalytic materials discovery.
Relying on recent results of the research group, and facing the state-of-the-art, ioChem-BD emerges as the ideal platform to build such those new tools around. In addition to the new raw data well-structured and that will be made publicly available in open form, additional open-source tools will be created that will implement advanced data analytics and artificial intelligence based predictive methods. Since all the data and services will be hosted by the Barcelona Supercomputer Center, this project will promote both the use of that infrastructure and data good practices among the community.

WORK PLAN



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