ioChem-BD: Tools for Open-Access Publishing and Much More …

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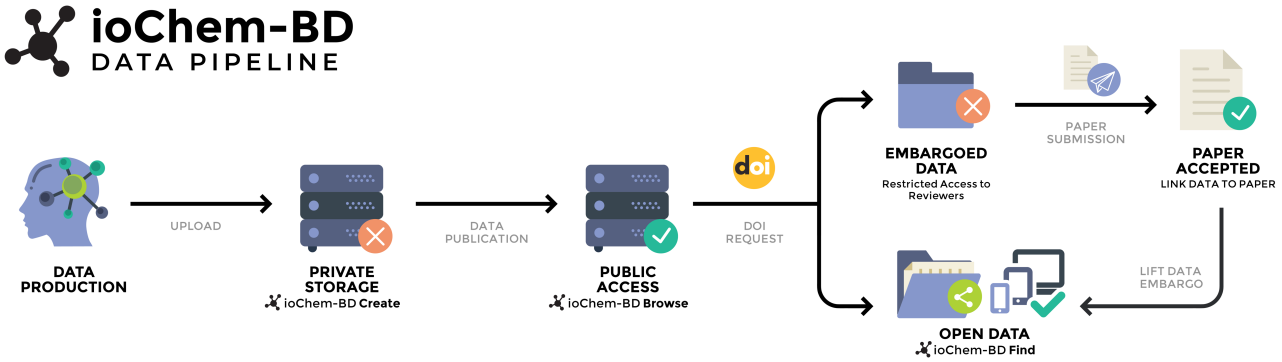
Scientific data needs to be properly stored and organized in order to meet Open Science requirements, which demand findable, accessible, interoperable and reusable (FAIR) data. Following these principles, ioChem-BD (www.iochem-bd.org) is a distributed platform of services aimed at helping researchers to manage their results, and to share them to the scientific community, promoting thereby the efficiency and sustainability in computational chemistry research. ioChem-BD deals with input and results files obtained from widely used codes, being Gaussian, VASP, ADF, Turbomole, Orca, Molcas, QuantumEspresso, and MOPAC currently supported. An independent modules architecture covers the whole data cycle, from data production to paper publishing by implementing a unique data pipeline (see Scheme).

The Central Point of our network of repositories, the Find service, is fed by ioChem-BD distributed nodes whenever a new item is published, provides advanced indexing of chemical data and metadata and a very fast search engine implemented over Apache Solr and RDKit frameworks, allowing queries by chemical substructure similarity, chemical elements or any text term.

Each ioChem-BD node implements services for private use of the data. In addition to visualization tools for reaction energy profiles, orbitals, spectra, etc ..., the Create module provides a REST API interface that enables remote interaction and processes automation. This presentation will showcase some examples of how to integrate ioChem-BD with Fireworks[2] for problem solving in catalysis and molecular modelling.[3]



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