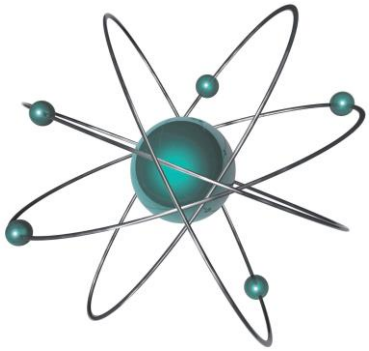
Reference Network on
Theoretical and Computational Chemistry



THE COMPUTATIONAL CHEMISTRY BIGDATA PLATFORM

The big amount of data resulting from scientific simulations needs to be properly stored and organized. The ioCHEM-BD[1] platform helps researchers to do so, and also allows sharing these results with the scientific community, promoting thereby the efficiency and sustainability in computational research.

ioChem-BD is a digital repository ideal to manage and to store computational chemistry input and results files obtained from chemistry codes, such as Gaussian, VASP, ADF, Turbomole, Orca, Molcas.

Numerical data is captured and translated into **XML/CML** code (Xtensible Markup Language for Chemical applications) by highly efficient converters. The XML data is visualized as HTML5 pages, allowing to access the generated molecules output information, such as geometries, energies, chemical or physical properties, and to manipulate them in an easy and configurable way. On the other side, it gets instantaneous visualization of different kind of spectra, orbitals, reaction energy profiles, geometries and many other properties.

The platform allows the user **to publish the converted data**, becoming an open access digital repository of computational chemistry results. Fully compliant Metadata (Dublin core) are added at publishing time for indexing. Published dataset collections are permanently indexed by means of DOI URL references, filling the gap between results generation and manuscript publication.

ioChem-BD is a very useful tool for reproducing results and for data harvesting.

Why should you use it?

The modular structure of the repository permits to perform a wide variety of duties such as:

- Improving the local data management, its search and its manipulation, keeping it safe and private.
- Making the data public in a controlled manner
- Browsing into published data, finding bibliography, results and molecules configurations.

Who is it aimed to?

- Academia Institutions
- Companies dealing with huge amount of data
- Software companies

Contact information

ICIQ Institut Català d'Investigació Química

contact@iochem-bd.org

info@xrqtc.com