

**21 months research fellow for the project “Computational re-design of mini iron-sulfur proteins for the activation of small molecules and for their conversion into value-added chemicals with energetic and environmental relevance.”**

Small molecule activation is a research area that is highly relevant from an energetic-environmental standpoint, since it allows to convert inert substrates into value-added chemicals, such as biofuels. In Nature, small molecule activation is mediated by several iron-sulfur metalloenzymes that operates under mild conditions and with outstanding rates. This makes them particularly attractive to develop sustainable strategies for energy carrier production. However, their high complexity makes a structural simplification strategy almost necessary. One strategy to do so, is the re-design of small and easy-to-handle proteins in order to transform them into active catalysts towards a specific task. In this context, this project regards the computational re-design of mini iron-sulfur proteins (Rieske, MitoNEET) in order to impart them catalytic activity towards the production of green hydrogen and other biofuels, for instance via carbon dioxide reduction. This will imply the use of molecular modelling tools (both in the quantum mechanics and molecular mechanics frameworks) as well as the development of predictive models in order to optimize specific relevant stereo-electronic features (redox potential, metal content) and catalytic activity.

Where: University of Milano-Bicocca, Biotechnology and Biosciences department

Start: March 2024

Contacts: [federica.arrigoni@unimib.it](mailto:federica.arrigoni@unimib.it); [giuseppe.zampella@unimib.it](mailto:giuseppe.zampella@unimib.it)

Candidate selection: January 2024

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