Biotechnology
and Biosciences
Seminars

Dipartimento di Biotecnologie e Bioscienze – UNIMIB

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Molecular Modeling serving bioinorganic catalysis: from metalloenzymes to designed biomimetic systems

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Abstract: Metalloenzymes can accomplish some of the most challenging chemical tasks, at outstanding rates, under mild conditions, with high selectivity, and by means of only cheap and bioavailable metal ions. For these reasons, they are considered a source of inspiration for the development of novel catalysts with tailored properties. The elusive and intrinsically complicated chemistry of transition metals makes the use of molecular modeling, at different levels of theory, fundamental for the rationalization of structure-reactivity relationships, of either metalloenzymes or their bio-inspired catalysts. I will present our most recent research in this context by showing, on the one hand, how different computational methods can address specific chemical problems and, on the other, which strategies can be followed to rationally design novel bio-inspired catalysts, such as homogeneous catalysts or de novo designed artificial metalloproteins.

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