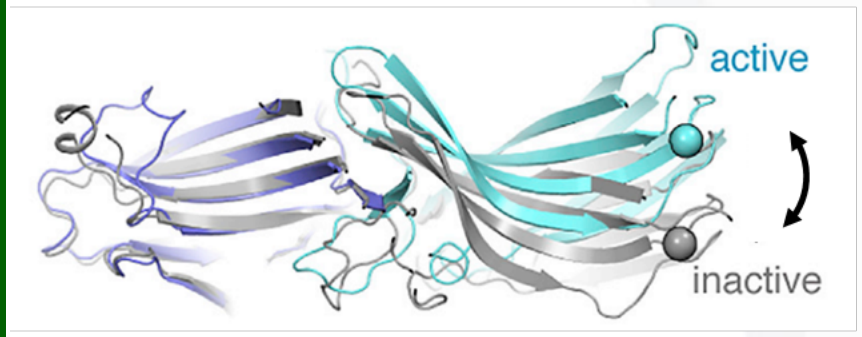
Luca Bertini – Federica Arrigoni – Giusepppe Zampella – Luca De Gioia
Laboratorio 4065 @ BTBS (luca.bertini@unimib.it)

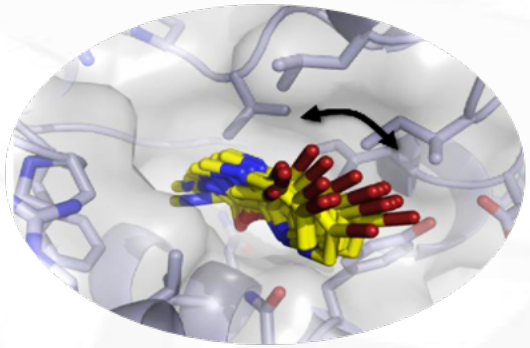
Progetti di Tesi 2023/2024

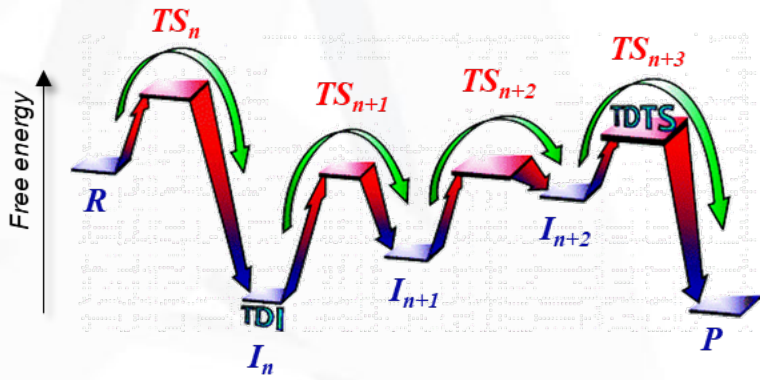
Modeling computazione e predizione delle proprietà di siti catalitici di metallo-enzimi

- Laccasi
- CYP152
- Idrogenasi

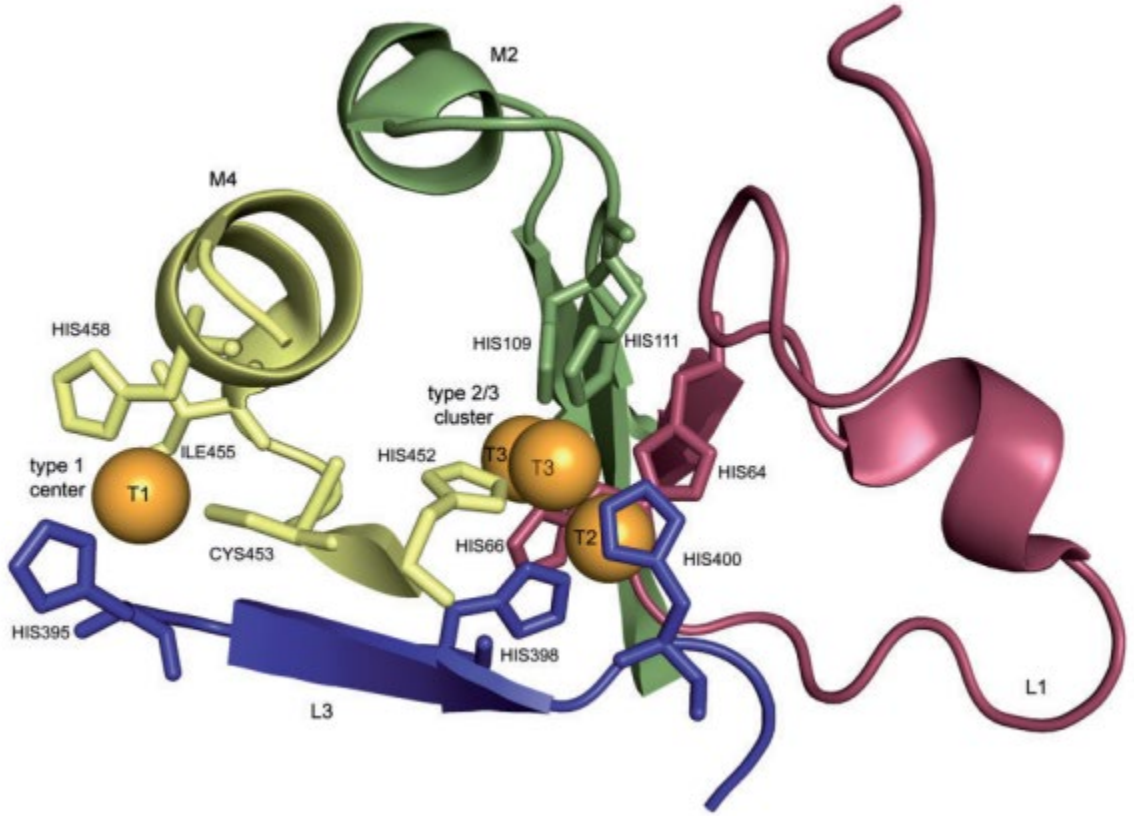
Modelling classico e quantistico



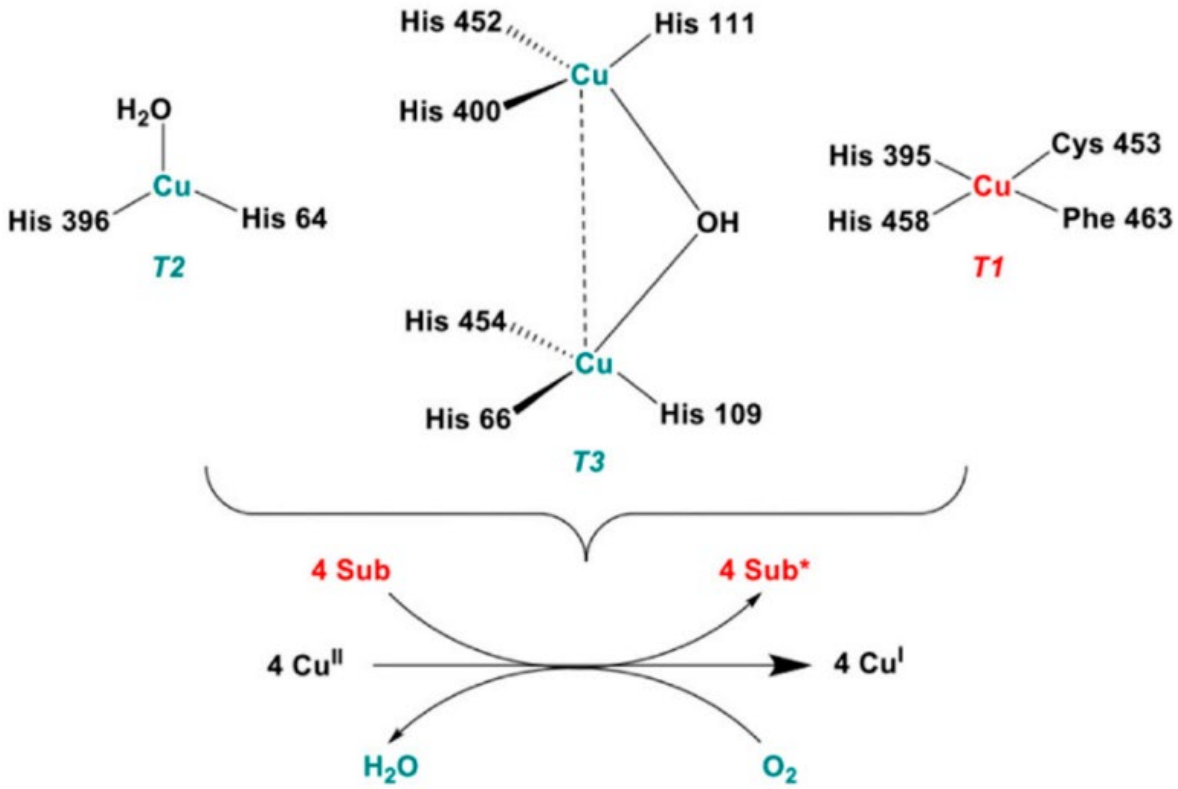




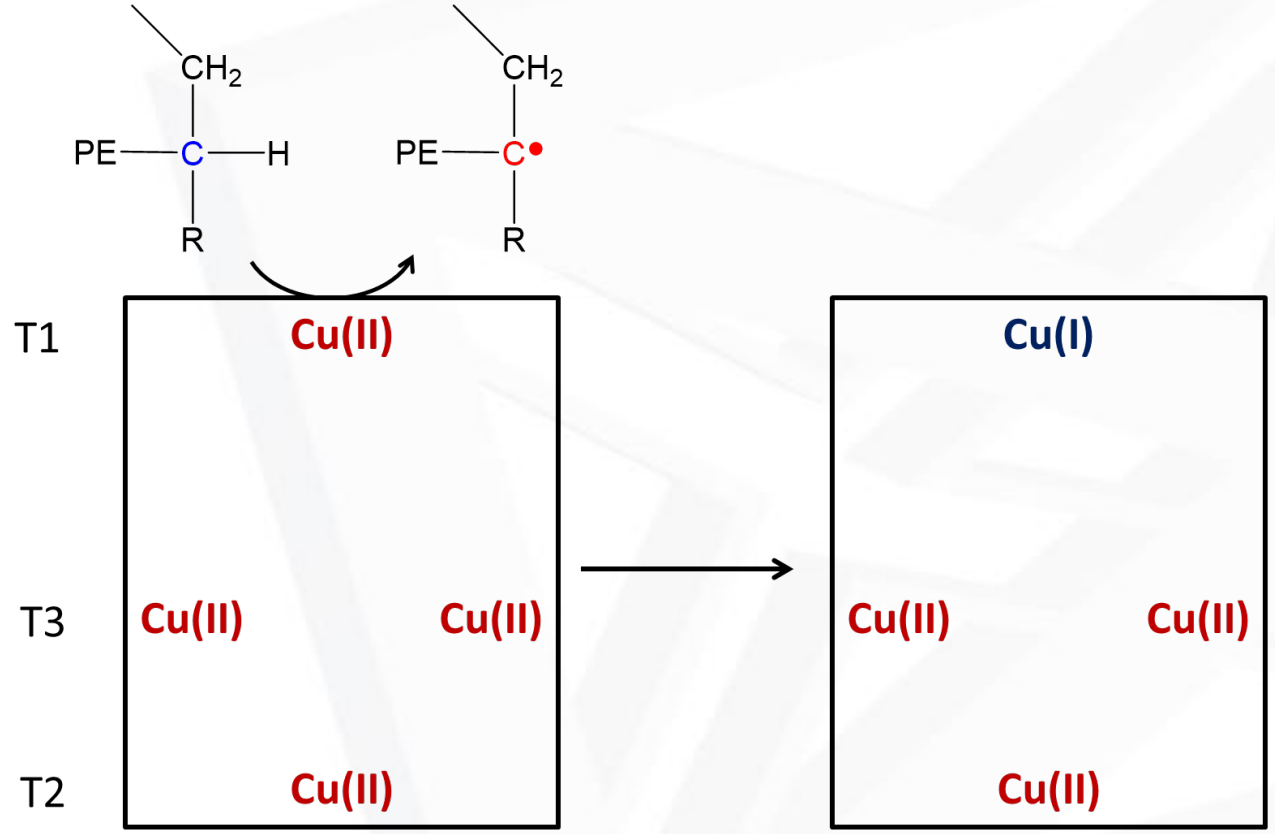
Laccasi batteriche e bioremediation



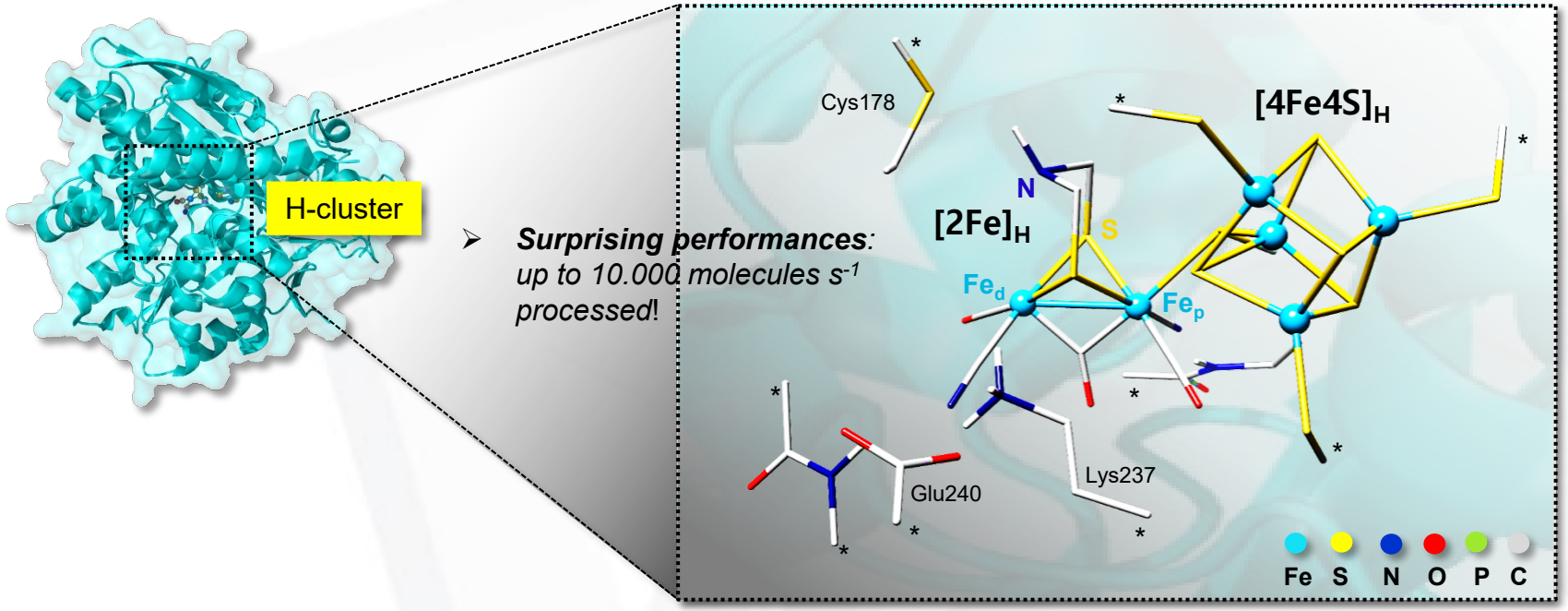
Laccasi batteriche e bioremediation



Laccasi batteriche e bioremediation



Idrogenasi



➢ ***Surprising performances**: up to 10.000 molecules s^{-1} processed!*

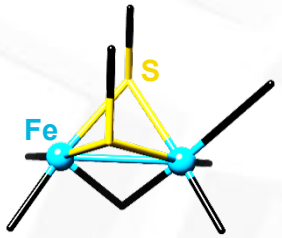
Idrogenasi

[FeFe]-HYDROGENASES

$H_2 \rightleftharpoons 2(H^+/e^-)$

ACTIVE SITE

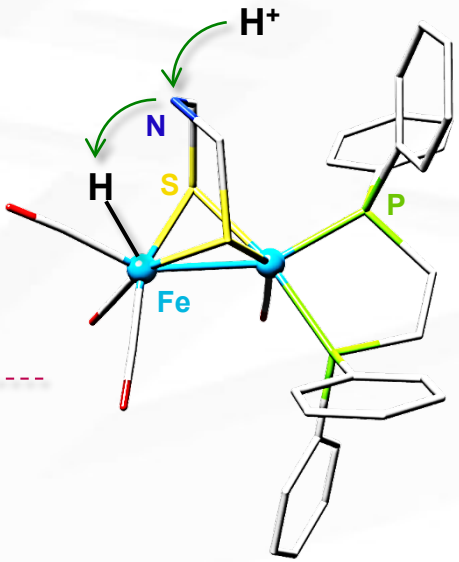
REACTIVE CORE



$[2Fe]_H$

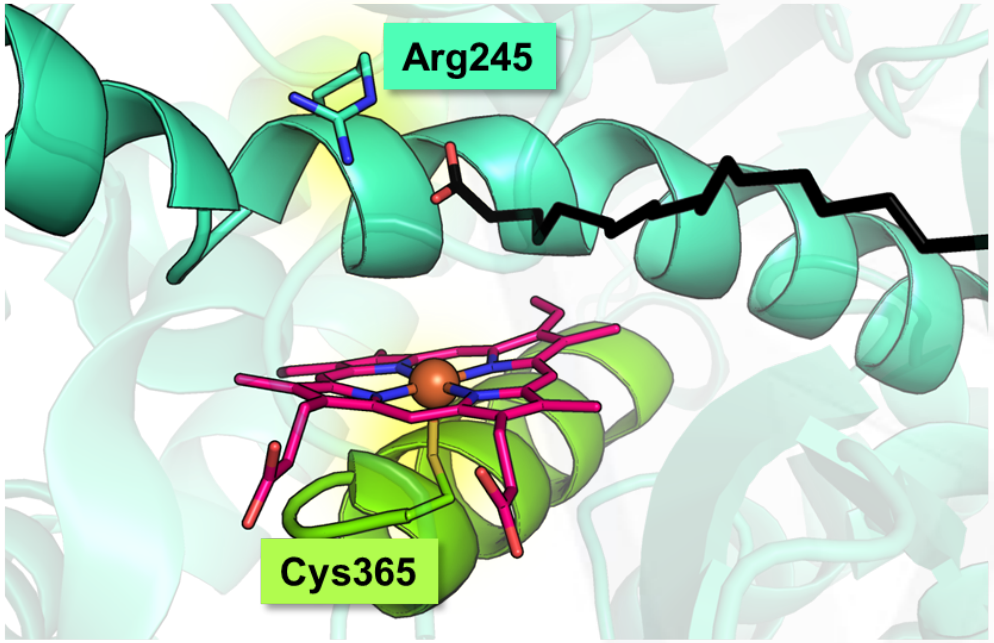
BIOMIMICS: Fe_2S_2 SYSTEMS

$H_2 \rightleftharpoons 2(H^+/e^-)$



- ***Lower performances*** than the natural system in the H_2 production direction

CYP152



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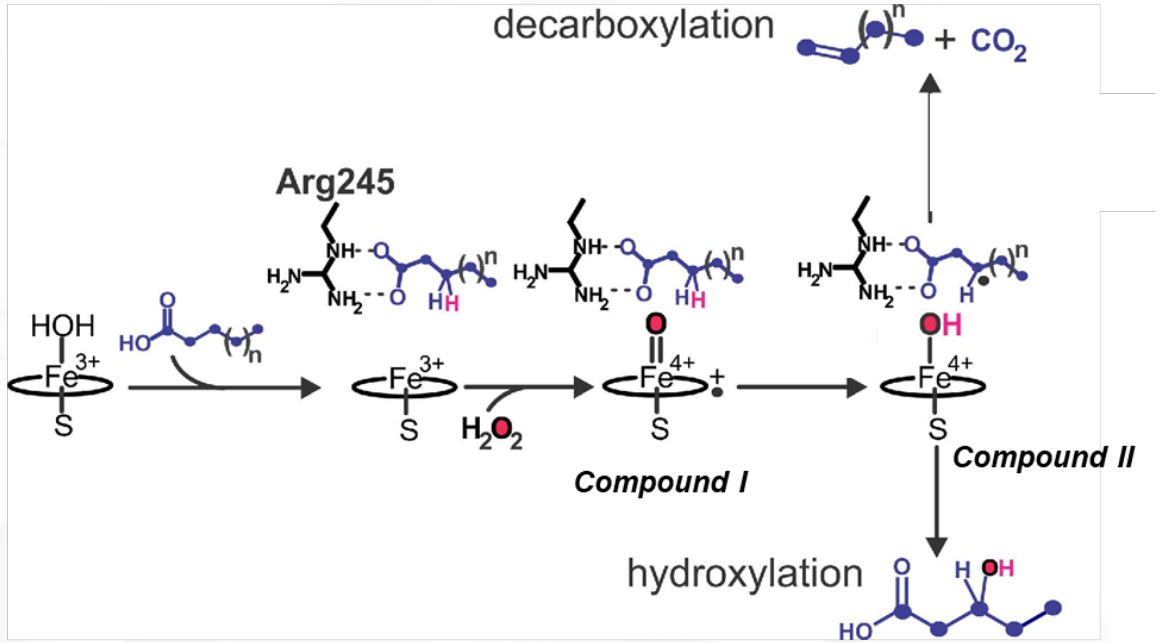

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