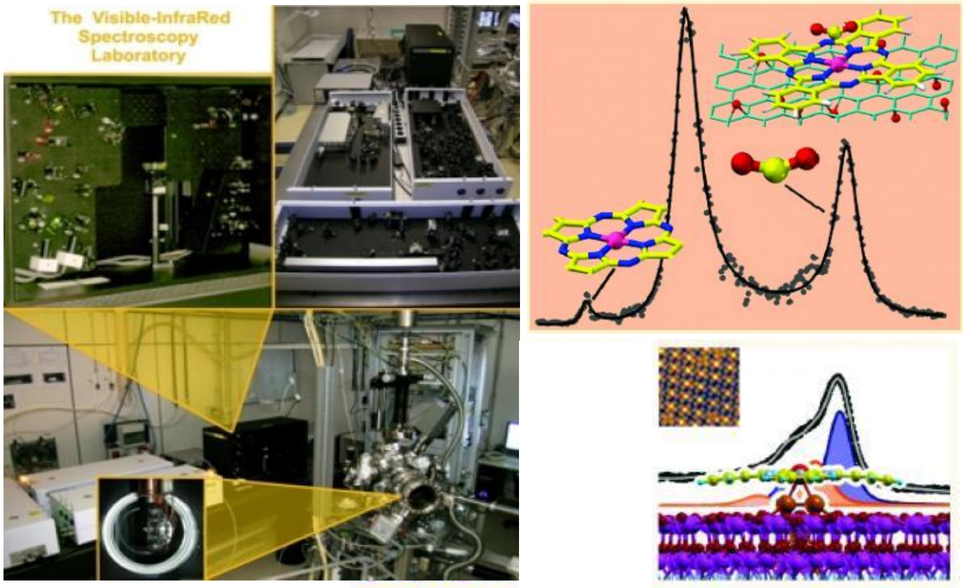
2D materials at near ambient pressure: a fundamental spectroscopic approach



Nature performs catalytic reactions for the synthesis of energy vectors and organic compounds by exploiting nano-sized or single-atom photosystem and enzymatic catalytic centers, where metals (Mn, Cu, Ni, Fe…) are supported by C, S, or N linkers. Light harvesting and funneling to electronic devices, storage, or reaction centers for chemical conversion is one of the biggest challenges to face in the view of a renewable and clean energy scenario. Technologically speaking, this translates in the search for optimal materials (in terms of low cost, high efficiency and sustainability) based on a detailed and thorough understanding of the involved physical processes in the framework of a bottom up approach. Charge transfer related to exciton dissociation (electron-hole separation), charge transport, delivery of energy to nano-engineered chemical reaction centers, and electron injection at the electrodes are indeed the rate limiting and crucial processes. The project will address new hybrid systems that combine the multifunctionalities of organic materials to those of 2D heterostructures. The interaction and reactivity properties of ordered, self-assembled metallorganic monolayers and 2D stacks (graphene, phosphorene, borophene) will be investigated *in situ* and *operando* by means of IR-Vis SFG vibronic spectroscopy and synchrotron radiation-based spectroscopies. We have already observed bonding of the reactants at nanostructured surfaces and with the single metal atom catalytic centers of an organic framework under biomimetic reaction conditions. The catalytic activity of proteins and enzymes in Nature for the storage or conversion of molecular reactants is indeed operative in the near-ambient partial pressure regime. Therefore, the IR-Vis SFG based experiments will provide *in situ* and *operando* insight into both vibrational and electronic properties of investigated 2D stacked systems. Optimal candidates are metal porphyrins and phthalocyanines supported on templates like graphene, borophene, or phosphorene, undergoing self-assembly into stable, ordered monolayers upon CVD.

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