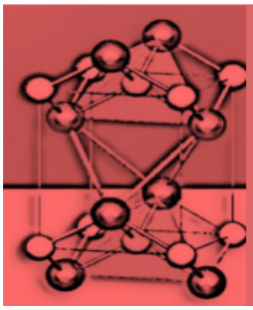

IX Workshop on Novel Methods for Electronic Structure Calculations

10th – 19th November 2021
La Plata – Argentina

Computer simulations of materials through ab-initio electronic structure calculations performed at IF-USP

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Some examples of the research actually performed in our group at IF-USP using ab initio electronic structure calculations in the framework of the Density Functional Theory in the Kohn-Sham scheme will be shown. We also use these ab-initio results as input to multiscale approaches to model and understand properties of advanced materials. Currently under study are electronic, magnetic, hyperfine and spectroscopic properties of materials with focus on nanomagnetism, hybrid improper ferroelectrics and systems with Nano-biotechnological applications.