Computational Materials Science from solid state physics to biochemistry

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Abstract: The common denominator of this general presentation about our research activities is the application (and development) of the most advanced computational tools in the field of molecular electronics, surface chemistry and biochemical reactions. For each case a short overview of the underlying theoretical framework will be given, before showing how nowadays computer modelling has become a practical tool to perform virtual experiments in a wide variety of fields at the crossroad among physics, chemistry, biology and engineering.
More specifically, molecular nanojunctions, patterning of graphene-based materials and proteins-RNA complexes will be used as representative examples of atomic-scale driven processes having a macroscopic impact in future technologies and life science.