SMART THEME: Surface-supported Molecular ARchiTectures: THEory Meets Experiment

The future of nano-electronics has been proposed to be switching soon from bulk 3D materials to lower dimensionalities.
The self-assembly of well-designed molecular precursors on appropriate surfaces is a very promising route towards 1D/2D materials with a high degree of long-range order and tailored functionalities. However, the synthesis of well controlled molecular networks is a lengthy and expensive trial-and-error process because growth driving forces are poorly understood and generally hard to investigate. Research in the field can be improved and sped up thanks to optimization guidelines derived from first principles modeling of the elemental steps of the growth process. This project aims to develop a synergistic theoretical and experimental line of research on the on-surface synthesis of novel surface-supported molecular architectures. The candidate is a well experienced computational quantum chemist which will integrate a team of experimentalists and theoreticians expert in the field of molecular assembling and reactivity at surfaces. Novel methods in density functional theory will be employed to simulate complex molecular configurations and reactions paths. On one side the theoretical activity will provide predictive modeling of the mechanisms of surface-assisted reactions and fundamental insights for the interpretation of microscopy and spectroscopy observations. On the other side, precisely targeted experiments will provide the necessary validation of the theoretical approaches employed and will stimulate the most pertinent directions over which the theoretical modeling should be addressed. The ultimate goal of the project will be to build an irreplaceable theoretical tool to rationalize experiments and to drive them towards optimal synthesis routes.

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Find out more: https://cordis.europa.eu/project/rcn/221805/factsheet/en