

# SUSTAINABLE MATERIALS, PROCESSES AND SYSTEMS FOR ENERGY TRANSITION

## MUR DM 118 - Computational design of molecular solar thermal fuels

<b>Funded By</b>	MINISTERO DELL'UNIVERSITA' E DELLA RICERCA [Piva/CF:97429780584] ALMA MATER STUDIORUM UNIVERSITA' DI BOLOGNA [Piva/CF:01131710376]
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<b>Context of the research activity</b>	<p>The project involves the development of a digital platform based on the combination of computational chemistry techniques and artificial intelligence to design new molecules and predict their physical properties relevant for their use as molecular solar thermal fuels. The development of this platform, in addition to contributing to the design of more efficient MOSTs, could be pioneering in the integration of digital technologies in the chemical sector.</p> <p>Progetto finanziato nell'ambito del PNRR – DM 118/2023 - CUP E14D23001840006</p>
<b>Objectives</b>	<p>Progetto finanziato nell'ambito del PNRR – DM 118/2023 - CUP E14D23001840006</p> <p>Main seat to carry out research: Department of Industrial Chemistry, University of Bologna, Viale Risorgimento 4, 40136 Bologna</p>
<b>Skills and competencies for the development of the activity</b>	<ul style="list-style-type: none"><li>- Graduate-level knowledge of physical chemistry, with particular focus on quantum mechanics</li><li>- Graduate-level knowledge of organic chemistry</li><li>- Basic knowledge of programming and scripting languages</li><li>- Expertise with quantum chemistry software</li></ul>