

Master in Photonics – “PHOTONICS BCN” Master ERASMUS Mundus “EuroPhotonics”

MASTER THESIS PROPOSAL

Dates: April 2021 - September 2022

Laboratory: CO2MAP, ICFO

ACCELERATED MATERIALS DISCOVERY

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Keywords: Nanomaterials, Nanotechnology, AI

Summary of the subject (maximum 1 page):

The discovery of new materials has fueled the most relevant technological advances across history. Advances in modern chemistry and physics, combined with nanotechnology have enabled a rapid growth in the knowledge and utilization of emerging materials, offering guidance into their design from the atomic level, synthesis, and discovery of new classes of materials.

There are virtually infinite combinations of materials in terms of composition and structure. To date, the discovery of new materials has been based on serendipity, empirical observations, or time-consuming computational modeling. In this project, we will utilize artificial intelligence to accelerate the design of new materials for energy harvesting and storage applications.

The prospective student will combine work on some of the next:

- Coding, data science, analysis, and artificial intelligence
- Computation modelling of materials
- Mechatronics, automation of synthesis and characterization
- Self-driven laboratories

Suggested literature:

<https://www.nature.com/articles/s41578-018-0005-z>