# CHEMICAL ENGINEERING

## AMMIN/DISAT - Multiscale digital design of crystalline particles and industrial crystallisation processes

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| **Funded By** | Dipartimento DISAT<br>Politecnico di TORINO [P.iva/CF:00518460019] |
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| **Context of the research activity** | Multiscale design of crystalline particles and industrial crystallization processes through the integration of molecular simulations, population balances, computational fluid dynamics, and experimental validation. The aim is to predict and control polymorphism, particle size, morphology, and the performance of the final product. |
| **Objectives** | Crystallization is a multiphase unit operation widely employed in the chemical, food, pharmaceutical, and agrochemical sectors. Crystal properties such as polymorphism, size distribution, and morphology have a decisive influence on the performance of the final product, including its solubility, bioaccessibility, and dissolution rate. Modeling nevertheless remains challenging because of the multicomponent and multiphase nature of the system and the interplay among phenomena that develop across the molecular, crystal, and process scales.<br><br>The project aims to develop a multiscale platform for the predictive design of crystallization processes for organic compounds. The platform will integrate molecular dynamics simulations and free energy calculations based on thermodynamic integration to describe solid-solvent interactions; population balance models to represent the evolution of the crystal size distribution; and computational fluid dynamics to quantify the effect of mixing and transport phenomena on nucleation, growth, aggregation, and breakage kinetics.<br><br>The originality of the proposal lies in the integration of these levels of description together with experimental validation. To this end, dedicated experimental activities will be carried out for the qualitative and quantitative investigation of crystallization kinetics, as well as for the advanced characterization of solids by means of synchrotron light tomography, atomic force microscopy, and nano-IR.<br><br>The project is multidisciplinary because it aims at developing advanced multiscale modeling approaches, validated through advanced experimental techniques. The expected impact is both scientific and industrial, through the |

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| | development of innovative methodologies and the acceleration of research and development in fields where control of crystalline properties is crucial. |

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| **Skills and competencies for the development of the activity** | Master’s degree in Chemical Engineering is required. Previous experience in modeling and/or experimental activities related to crystallization is highly desirable. |