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Machine learning of molecular motifs in soft supramolecular systems

By

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Machine learning of molecular motifs in soft supramolecular systems

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Defects are ubiquitous in our world and they forcefully populate every aspect of our life. Although, defects are often random and sporadic, making them challenging to detect and quantify, they can also provide valuable insight into properties and behavior of materials. Within the field of materials science, defects play a central role, driving a huge plethora of phenomena. However, to this day, we are still missing a comprehensive and general theory on how to systematically detect and learn how to control defects, especially in soft-matter systems. In modern days, following the improvements in several technological areas, we are acquiring new tools that can help scientists to better understand and rationalize elusive phenomena, such as the complex structural dynamic behavior of some soft materials. Recently, Machine Learning (ML) techniques are gaining a lot of popularity, as they can decompose virtually anything in mathematical entities, which can later be used as a baseline to formulate new theories, explain trends and/or draw data-driven conclusions. The work presented herein focuses on a variety of soft self-assembled systems that posses an intrinsic structural and dynamical complexity (*e.g.*, supramolecular fibres, micellar aggregates, bilayers and nanoparticles) and on how to compare, classify and control them. In this sense, a universal workflow is proposed and discussed, suitable for the complete structural description and comparison of various soft materials, focusing on the concept of structural defects as common ground. The work I have conducted builds on the concept that defects, which actively populate such assemblies, determine and influence their structural and dynamical features. However, detecting such entities in a unambiguous and unbiased way is not an easy task. Using machine learning based tools we developed a data-driven "defectometer", an analysis tool, that can be employed to compare and characterize virtually all kind of supramolecular structures, based on their intrinsic "defectivity". We believe that this represents a first step towards the rational design and engineering of new types of materials with controllable structural features.