THE SYNERGY OF CRYSTALLOGRAPHY AND THEORETICAL INVESTIGATIONS

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The crystallography plays a very important role for science and human life due the fact that allows the study of the structure of matter at the atomic or molecular level, based on this knowledge, opening the possibility for the development of new drugs and more efficient materials. Crystallography involves multidisciplinary problems and attracts researchers from different areas, estimated that the 45 Nobel winners in the last decades, in the areas of physiology, biology, chemistry and physics are related to crystallography. Theoretical predictions based on quantum theory contributed meaningfully with crystallographic data to analysis of the diverse intermolecular interactions and properties of new materials. Understanding how intermolecular interactions lead to crystal formation is fundamental for supramolecular chemistry and crystal engineering. The knowledge generated by these methods helps to understand the crystalline state of materials, produces advances for basic science and for industry, considering that, from this information, atomic and molecular engineering will be able to manipulate them in a way that a new industrial revolution with important economic and environmental consequences may arise. There is an intimate relationship between the three-dimensional structure of proteins and their function. Each fold in protein is driven by a series of non-covalent interactions, such as hydrogen bonds, ionic interactions, Van der Waals forces, and hydrophobic packing. Knowing the structure of a protein it's possible to find or design small chemical compounds that fit together in ways that selectively modulate protein functions for example. Another point is ensured that the drug has not undergone any polymorphic transition because its changes their bioavailability, as well as the dissolution rate and absorption. Another important contribution of crystallography and quantum mechanics is the research of new materials with high linear and nonlinear optical properties. In this point, theoretical calculations based in quantum mechanics speed up the search for new crystalline structures with desired properties. These are just some areas where crystallography and quantum mechanics can supply the international perspectives related to critical need, such as medicines and raw materials for products which lead to improved quality of life. This summary indicates crystallography and computer simulations based on quantum calculations as two methodologies capable of providing a rigorous analysis of intermolecular interactions The synergy of crystallography and quantum mechanics have great potential to contributed to a wide range of studies going to meet the most diverse human needs and allowing the design of new molecular solids with desired properties and functions.

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