



Crystals As Giant Molecules (Lecture Notes in Chemistry, Vol 9)

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Traditionally, when one deals with crystals, the first property to be presented is the periodicity of the lattice, and all methods of study are based on this characteristic, which is considered essential. In fact, crystals differ from the molecules of finite size that are studied in chemistry, only in their extremely large number of particles. Furthermore, the existence of faces, which limit the spread of crystals in space, necessarily breaks the periodicity of the system. For these reasons it is natural to apply to crystals the concepts and methods that have been widely tested in the study of molecules. Pauling first emphasized this point 1 and used it to explain the electronic structure of crystals, thought to be infinite and perfect. The aim of this work is to show, with the help of a few examples, the possibilities offered by quantum chemistry for tackling the problems of crystal electronic structure, of crystallographic arrangements as well as their macroscopic shape, and of distortion effects caused by the presence of faces. The area related to the existence of energy bands (allowed or forbidden), gap, electric, magnetic or optical properties will not be touched upon.

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