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Sommario/riassunto	Unravelling an intricate network of interatomic interactions and their relations to different behaviors of chemical compounds is key to the successful design of new materials for both existing and novel applications, from medicine to innovative concepts of molecular electronics and spintronics. X-ray crystallography has proven to be very helpful in addressing many important chemical problems in modern materials science and biosciences. Intertwined with computational techniques, it provides insights into the nature of chemical bonding and the physicochemical properties (including optical, magnetic, electrical, mechanical, and others) of crystalline materials, otherwise accessible by experimental techniques that are not so readily available to chemists. In addition to the advanced approaches in charge density analysis made possible by X-ray diffraction, the information collected over the years through this technique (which is easily mined from huge databases) has tremendous use in the design of new materials for medicine, gas storage, and separation applications as well as for electronic devices. This Special Issue contains two reviews and five articles that cover very different aspects of ‘composition–structure’ and ‘structure–property’ relations identified by X-ray diffraction and complementary techniques (from conventional IR and Raman spectroscopies to cutting-edge quantum chemical calculations) and their use in crystal engineering and materials science.