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Sommario/riassunto	<p>The term “first-principles calculations” is a synonym for the numerical determination of the electronic structure of atoms, molecules, clusters, or materials from ‘first principles’, i.e., without any approximations to the underlying quantum-mechanical equations. Although numerous approximate approaches have been developed for small molecular systems since the late 1920s, it was not until the advent of the density functional theory (DFT) in the 1960s that accurate “first-principles” calculations could be conducted for crystalline materials. The rapid development of this method over the past two decades allowed it to evolve from an explanatory to a truly predictive tool. Yet, challenges remain: complex chemical compositions, variable external conditions (such as pressure), defects, or properties that rely on collective excitations—all represent computational and/or methodological bottlenecks. This Special Issue comprises a collection of papers that use DFT to tackle some of these challenges and thus highlight what can (and cannot yet) be achieved using first-principles calculations of crystals.</p>