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Conceptual and Computational Progress in Modeling Materials

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Advances in modeling material systems since the development of quantum mechanics in the 1920s came much slower than progress in unraveling the electronic structure of atoms. This is particularly evident when one compares the identification of spectral features. For atomic spectra, lines are sharp and identification in terms of electronic transitions is much easier than for the case of solids where spectral features are generally broad. At first, empirical approaches paved the way, and eventually, it became possible to explain electronic and structural properties of fairly complex solids from first principles using only information about their constituent atoms as input. Because of the central role of electronic structure in understanding bonding and other properties, much of the focus has been on obtaining band structures and electron density maps. Eventually, this led to accurate determinations of ground-state mechanical and vibrational properties. In fact, at this time, ground-state calculations are of high precision and have been extended to compute electron-lattice interactions. In turn, these are used to explain and predict superconductivity in materials and to provide detailed calculations of superconducting properties. The model used for much of this work is based on pseudopotentials and density functional theory. It is sometimes referred to as the "Standard Model of Solids". The approach is a result of the development of many new conceptual models and the great progress in computation.