The spatial arrangement of atoms in a crystalline solid can be determined very precisely by modern analysis methods. It is, however, rarely possible to deduce the driving forces for a certain arrangement from the experimental data and to evolve relations to chemical concepts like covalency, charge transfer and van der Waals interactions. In metallic compounds a conceptual bonding analysis is even more complex, as the subdivision of the entirety of valence electrons into localized and delocalized parts is not obvious. On the other hand, the derivation of bonding properties from quantum mechanical calculations comprises certain arbitrariness. The bonding picture developed from the theoretical data in any case has to be in conformance with the measured properties.

The complex of problems is discussed by means of some examples:

1. Platinides contain an anionic Pt substructure. The fraction of itinerant electrons and the dimensionality of the anionic substructure depend on the number of electrons provided by the cations.
2. The structures of the group 12 elements deviate considerably from a close packing. Electronic correlation with a significant involvement of the filled d-shell is responsible for these deviations.
3. Some crystal structures are difficult to understand on the basis of standard electron counting rules. The assumption of localized electrons in polyhedral voids of the cationic partial structure resolves these difficulties.