

Bonds, symmetry and virtual atoms.

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An atom is only real when it is not bonded to other atoms. Once it is bonded it becomes a virtual atom because its properties are no longer unique but depend on how the atom is defined. QTAIM defines atomic fragments that are charged, but it is simpler to define bonded atoms to be identical to the uncharged free-atom. Placing such atoms at the observed positions of their nuclei gives the promolecule charge density which is a good approximation to the observed charge density. A bond is formed when two such atoms overlap, and simple electrostatic theory shows that only the charge in the overlap region attracts both atomic cores. This attraction can be represented by Faraday lines of field, the number of such lines being the electrostatic bond flux, which is the same as the bond valence that fully characterizes the bond. It correlates with both the bond length and the charge density at the bond critical point. The flux model predicts the structure, geometry and chemical reactivity of the resulting compound. No need to worry about ionicity or covalency, charge transfer, oxidation states, electron pair bonds, or orbitals. This classical description of the physics of the bond leads naturally to the traditional atom-bond, ionic and VSEPR models. It is consistent with, but complementary to, the quantum picture of the atom.