

Poster Presentation

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The Physical Origins of the Chemical Bond

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The properties of the chemical bond are the same as those of the electrostatic flux that links the cores of two bonded atoms via their bonding electrons. Both the bond and the flux depend only on the number of electrons that form the bond, and significantly, neither depends on how the electron density is distributed. This allows the rules of chemical bonding to be developed using classical electrostatic theory without the need to know how the electron density is distributed. The magnitude of the flux is equal to the bond order (bond valence) and hence correlates with the bond length [1]. A network of bonds is equivalent to a capacitive electric circuit which allows one to predict the bond fluxes, hence also the bond lengths. Bond angles are determined by the spherical symmetry of the flux around each atom, and the resulting bonding geometry can be predicted using little more than a pocket calculator. The rules of all the predictive bond models: the VSEPR model, the ionic model, the covalent bond model and the bond valence model can be derived using classical electrostatics without introducing problematic concepts such as hypervalency, dative bonding, hybridization and the dichotomy between ionic and covalent bonding, thus eliminating the paradoxes created by the physically questionable Lewis and orbital models. Quantum effects are rarely important except in the transition metals where in some cases they perturb the bonding geometry.

[1] C.Preiser, J.Loesel, I.D.Brown, M.Kunz and A.Skowron *Acta Cryst.* 1999, B55 698-711.

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