Quantum Mechanical Basis of Conceptual Chemistry

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Science is observation, experiment and theory. This is the path that led to the development of the molecular structure hypothesis - that a molecule is a collection atoms with characteristic properties linked by a network of bonds that impart a structure – a concept forged in the crucible of nineteenth century experimental chemistry. One hundred and fifty years of *experimental* chemistry underlie the realization that the properties of some total system, molecule or crystal, are the sum of its atomic contributions. The lecture will demonstrate that this conceptual basis of chemistry is recovered in its entirety by the Quantum Theory of Atoms in Molecules, [1] a theory grounded in the quantum mechanics of an open system and given physical expression in terms of a system's measurable [2] charge distribution.

[1] Bader R. F. W., "Atoms in Molecules: A Quantum Theory", Oxford University Press, Oxford UK, 1990. [2] Coppens, P., "X-Ray Charge Densities and Chemical Bonding", IUCR Texts on Crystallography.4. Oxford University Press, Oxford UK, 1997.

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