Towards Complementary Characterization of the Chemical Bond

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A precise discussion of a single bond requires consideration of two-particle wave function for the particles involved. Here we define and determine rigorously the intrinsic covalency and connected characteristics on the canonical example of H_2 molecule. This is achieved by starting from analytic form for the two–particle wave function for electrons forming the bond, in which we single out the atomic contribution (atomicity) in an unequivocal manner. The presence the of atomicity and ionicity factors complements the existing attributes of the bond. In this way, a gradual evolution of the molecular state to its two-atomic correspondent is traced down systematically with increasing interatomic distance. In effect, a direct relation to the onset of incipient Mott-Hubbard atomicity (Mottness) to the intrinsic covalency and ionicity is established. This goal is achieved by combining the single–particle wave function readjustment with a simultaneous determination of two–particle states in the particle (second – quantization) representation

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