Abstract Submitted
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Quantum-mechanical definition of atoms and their interactions in molecules[1] PETER LANGHOFF, University of California San Diego, MICHAL BEN-NUN, Predictive Science Inc, JEFFREY MILLS, JERRY BOATZ, Air Force Research Laboratory, GORDON GALLUP, University of Nebraska Lincoln — Assignments of indistinguishable electrons to particular atomic nuclei in a molecule are generally regarded as meaningless, as are associated definitions of fragment atomic and atomic-interaction operators. As a consequence, a generally agreed upon quantum-mechanical definition of a "chemical bond" between atoms in a molecule is largely absent. In the present report, a computationally-viable quantum-mechanical definition of chemical bonding between atoms in a molecule is presented based on the Born-Oppenheimer approximation, the Couloumb Hamiltonian operator, and the conditional context afforded by representation theory. An orthonormal (Eisenschitz-London) outer product of atomic spectral eigenstates is employed to provide meaningful assignments of electrons to particular atomic nuclei in a molecule, as well as support of corresponding well-defined self-adjoint atomic and atomic-interaction fragment operators. Total molecular energies obtained in this representation are partitioned into a sum of atomic terms which describe distributions of atomic energy promotions for the individual atoms and a pairwise-atomic sum of distributions among universal interaction energies which describe chemical bonds among the constituent atoms. Illustrative clarifying applications are reported.

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