A CONCEPT OF EFFECTIVE STATE OF ATOMS-IN-COMPOUNDS TO DESCRIBE PROPERTIES DETERMINED BY THE VALENCE ELECTRON'S DENSITIES IN ATOMIC CORES

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A new method of circumscribing the effective electronic states of "atoms-in-compounds" to study the properties of molecules and solids which are described by the operators heavily concentrated in atomic cores is discussed. Among the properties are hyperfine structure, P,T-parity nonconservation effects[b], chemical shifts of X-ray emission[c] and Mössbauer lines, etc. Advantage of the approach is that a good quantitative agreement of predicted and experimental data can be attained. From computational point of view the method is based on the relativistic pseudopotential theory [d] and procedures of a posteriori recovery of wave functions (which are smoothed near atomic nuclei at the molecular calculation stage with using the pseudopotential method) in the atomic cores. We report results of our recent investigations of a number of diatomic molecules.

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