Theoretical and Interpretative Paradoxa of Different Relativistic and Quasirelativistic Approaches

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The standard ab-initio approach in relativistic quantum chemistry rests on the Dirac equation, using the standard four-component spinor representation in ordinary (position or momentum) space. Then, r denotes the position of charge, and p=-id/dr the mass momentum. By unitary transformations one can pass over to effective Hamiltonians, to two-component representations, to pseudopotential or to one-component approximations. Thereby the expressions for expectation values, for the charge distribution, for the optical transition moment, for spin-orbit coupling etc., and the expressions for relativistic corrections change. Accordingly one must be careful when interpreting relativistic changes of structure, forces and energy of molecules. They may be explained through changes in the valence shell or in the inner core, using relativistically corrected or nonrelativistic wavefunctions, using forces or energy gradients. Combining different paradoxical viewpoints yield a clearer understanding of the mechanism of relativistic corrections.