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The first step in solving a quantum chemical problem is usually solving the Schrödinger equation (or Dirac equation in relativistic quantum chemistry) with the electronic molecular Hamiltonian.

Quantum chemistry - Wikipedia

A Brief Review of Elementary Quantum Chemistry C. David Sherrill School of Chemistry and Biochemistry Georgia Institute of Technology Last Revised on 27 January 2001

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Relativistic quantum chemistry combines relativistic mechanics with quantum chemistry to explain elemental properties and structure, especially for the heavier elements of the periodic table.

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