WANTED

Erwin Schrödinger

DEAD AND ALIVE

$$H\Psi = E\Psi$$

Born-Oppenheimer-Approximation

HF-SCF

Basisset

Post-HF

DHF Rel. PSP

Elektronen Correlation

Rel. Effects

Structure

Frequencies

Experiment

Energy

+

Optimized Wave function

Population Analyses

Chemical Interpretation