

Research fields

New methods development in:
Quantum chemistry and physics
Many-electron theory

- Electron correlation
- Density Functional Theory - development of the new correct exchange- correlation functionals and potentials
- Orbital dependent exchange and correlation functionals and potentials
- Optimized Effective Potential Method (OEP)
- Ab initio DFT
- Coupled Cluster Method
- Many-Body Perturbation Theory
- Connections between WFT and DFT
- Non-covalent interactions
- Numerical Methods in quantum chemistry and physics.
- Tensor Contraction Engine (TCE) and its applications in quantum chemistry.
- Computer systems and electronic data safety...