Research fields

New methods development in
quantum chemistry and physics
Many-electron theory

- Electron correlation
- Density Functional Theory
- Orbital dependent functionals and potentials
- Optimized Effective Potential Method (OEP)
- Coupled Cluster Method
- Many-Body Perturbation Theory
- Spina-Scaled-Component MP2 method
- Non-covalently interacting systems

- development of the new correct exchange- correlation functionals and potentials in DFT
- Ab initio DFT
- Orbital dependent exchange and correlation functionals and potentials
- Many-Body Perturbation Theory
- Connections between WFT and DFT
- Numerical Methods in quantum chemistry and physics.
- Tensor Contraction Engine (TCE) and its applications in quantum chemistry.
- Computer systems and electronic data safety