Analysis of materials:

- Materials and inorganic compounds (including metals, ceramics, oxides)
- Organics (including polymers)
- Biological compounds including proteins and enzymes
- Liquids, gases and solids

Type of calculations:

- Optimization of geometry: local minimum, global minimum, transition states
- Calculation of atom charge, length and bond order
- Conformational analysis
- Calculation of thermodynamic properties: enthalpy, entropy, free energy, heat of formation
- Calculation and visualization of molecular orbitals
- Calculation and analysis of IR, UV-VIS and NMR
- Calculation of dipole and quadrupole moments of molecules, as well as (hyper) polarizabilities
- Simulation of time-dependent phenomena
- Build and apply ADMET Models with QSAR

Computational methods:

- DFT: D-VWN, D-PW92, B88-PW91, PW91-PW91, B88-P86, B88-LYP
- Orbital Basis: 3-21G, 3-21G(p), 6-31G, 6-31G(p), 6-31G(p,d), DZVP, TZVP
- Semi-empirical methods: MINDO/3, MNDO, MNDO/d, AM1, PM3, PM5, PM6, RM1, PDDG/MNDO, PDDG/PM3, ZINDO, INDO/S, CNDO/S, CNDO/S2, CNDO/S3, CNDO/1, CNDO/2, INDO/1, INDO/2
- Linear-scaling semi-empirical methods for proteins and large biological systems
- Solvation models (COSMO model, Onsager model)
- Molecular Mechanics: MM2, MM3
- Molecular dynamics:
    - The use of external fields: Stress, Gravitational, Magnetic, Electric, Containing Sphere
    - Temperature and pressure-controlled during MD simulations
    - Addition of atoms / molecules the system during the simulation
    - Potentials (force fields) library:
        - Organic: AMBER, CC, Dreiding, KKY, Klein-McDonald, Organic, MM2, MOMEC, OPLS, SPC, TIP
        - Inorganic:
            - 2-Body: Born-Mayer-Huggins, Erkoc, Johnson, Kawamura, Lennard-Jones, Morse.
            - 3-Body: Justo, Marks, Stillinger-Weber, Tersoff.
            - Many-body: Ackland, Finnis-Sinclair, Grujicic-Zhou, long range Finnis-Sinclair, Oh-Johnson, RosatoGuillop-Legrand, tight binding, Voter-Chen, Yang-Johnson
        - Metallic materials: EAM: GEAM, MEAM
        - Ceramics: Tersoff, Finnis-Sinclair
        - Others: CFF, UFF.
    - Variable-charge potential

Excellent integrated Graphical User Interface with the following functionality:

- Creation of molecules, visualization of results, running calculations from graphical interface
- Creation and analyze of proteins: sequence, topology, analysis of the active center
- Automatic docking and 'scoring' of ligands to the active site of the protein
- Interface for automated calculations on large libraries of molecules with the ability to create of QSAR/QSPR models
- Support of 3D displays for stereographic molecule representation
- Model building and preparation of simulation cell at the molecular dynamics level by using:
    - tools for drawing molecules 2D / 3D
    - tools for system relaxation
    - tools for creating of unit cells for different systems: crystals, amorphous solids, polymers, dendrimers, liquid crystals, liquids, colloids, mixture of chemical compounds in the liquid and gas phase
    - tools for creating clusters, defects, interfaces
    - tools for the analysis of surface phenomena, such as adsorption, absorption, high-energy particles strike
- Analysis Modules for Molecular Dynamics simulations:
    - Motion Analysis of system components
    - Module that shows 2D graphs of temperature, pressure, internal energy, kinetic and potential energies, thermal conductivity and other thermodynamic properties varying as a function of time
    - Module that calculates the mean square displacement (MSD) from the output data. It also displays a 2D graph of the MSD, and the self-diffusion coefficient of each molecule.
    - Module that calculates the pair correlation function, radial distribution function, and running integration number, and displays the corresponding 2D graphs.
    - Internal coordinate module, which calculates and displays the distribution of geometrical properties of molecules in a histogram.
    - Module, which calculates modulus of elasticity from the fluctuation formula.
    - Module, which calculates density, crystal cell unit, self-diffusion coefficient, static dielectric constant, isothermal compressibility, and shear viscosity.
    - Module, which calculates the number of Voronoi polyhedra and the number of faces (polygons) of Voronoi polyhedra.
    - The possibility of calculation of the thermal conductivity of materials

SCIGRESS can transparently run and visualize results from the third party programs (external engines):

- Amsterdam Modeling Suite
- AutoDock (Vina and Tools)
- CONFLEX
- GAMESS
- Gaussian
- LAMMPS
- MOPAC
- Quantum ESPRESSO

SCIGRESS can read following file formats:

- LAMMPS: *.dmp
- Quantum ESPRESSO Molecular Dynamics: *.md.out
- Protein Databank: *.pdb, *.ent
- Tripos: *.mol2
- MDL: *.mol, *.mdl, *.sdf, *.sd
- XMol XYZ: *.xyz
- ShelX: *.ins
- Crystallographic Information: *.cif
- GAMESS: *.log
- MOPAC: *.mop, *.dat, *.out
- Gaussian: *.fch, *.fchk

Hardware and software configuration for desktop version:

- Minimum hardware configuration
  - Intel Pentium 4 2.0 GHz; 4 GB RAM; 250 MB HDD; OpenGL accelerated graphics hardware
- Operating systems:
  - Windows 7, 8, 10 - 64 bit
  - Linux - Ubuntu, OpenSUSE, Debian, Centos - 64 bit
  - MacOS - OS X 10.9 and higher

Hardware and software configuration for SCIGRESS Server:

- Java Runtime Environment is required, either version 7 or 8 would work.
- SSH server is needed to access SCIGRESS server and for file transfer.
- For 64-bits version of Linux, 32-bits compatibility libraries need to be installed. In particular, 32-bits glibc and libstdc++.so.6 are needed.

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