THE USE OF COMPUTER-ASSISTED MOLECULAR MODELING IN COURSE OF STUDY "QUANTUM CHEMISTRY"

Yurchenko O., *Korolchuk S., Kormosh Z., Savchuk T.*
Lesya Ukrainka Volyn National University
43025, Lutsk, 13? Voli Avenue
yurchenko.oksana@vnu.edu.ua

One of the tasks of computational quantum chemistry is to determine the structure and properties of chemical compounds, reactivity, kinetics and the mechanism of chemical reactions based on quantum mechanics. For most quantum chemical systems, it is impossible to find exact solutions; therefore, approximate calculation methods are used.

To find the structure and properties of molecules, molecular modeling is used - various computational methods with subsequent visualization of the results, providing their three-dimensional representation under the conditions specified in the calculation

Molecular modeling methods are used in computer chemistry, materials science, and biology to study both individual molecules and interactions in molecular systems.

The amount of computations in the simulation of systems of practical interest, especially in the study of molecular dynamics, is very large and difficult to carry out manually. As a result, computer methods of calculation and visualization are used. This technique is called computer-assisted molecular modeling (CAMM).

There are many programs for computer-assisted molecular modeling [ADF, Agile Molecule, Avogadro, Cerius2, GAUSSIAN, Ghemical, GROMACS, etc.). Some programs are free, some are commercial.

Let's consider the most common and reliably tested programs for quantum chemical calculations. These include GAMESS, GAUSSIAN, HyperChem.

Gaussian is a software package for calculating the structure and properties of molecular systems in the gas-phase and condensed state, including a wide variety of methods of computational chemistry, quantum chemistry, and molecular modeling. Created by Nobel laureate John Popl and his research team and has been constantly updated since then. Allows you to calculate a large number of molecular properties, including structure, energy, thermodynamic characteristics, vibrational frequencies, energies of electronic excitations, properties of molecules in excited states, the influence of the environment and other properties. It includes the implementation of many methods for calculating the structures and properties of molecules, for example, methods such as: DFT, AMBER, AM1, PM3, ONIOM, etc. The program also allows you to generate so-called cube files, which can be used by many programs for visualizing molecular systems. Gaussian is one of the most powerful and perhaps the most widely used package for solving these problems. The program has a user-friendly interface. Disadvantages of the program: only works in English; there is a commercial program; it is necessary to visualize the output files using a visualizer program (Gauss View).

GaussView is a graphical interface for Gaussian that allows you to process and visualize the results of calculations. The program allows you to visualize, for example, optimized molecular structures, molecular orbitals, atomic charges and dipole moments, and much more.

GAMESS (General Atomic and Molecular Electronic Structure System) - general-purpose program for calculating atomic and molecular structures. There are three main flavors of the program supported by different groups: GAMESS US, GAMESS UK, and Firefly (PC GAMESS), which differ slightly in their capabilities. The Firefly version was developed at Moscow State University (by A. Granovsky). In this program it is possible:

1.Calculation of molecular wave functions by the self-consistent field method in the RHF, UHF, ROHF, GVB and MCSCF approximations;

2.Accounting for electron correlation energy based on perturbation theory, configuration interaction, coupled clusters and density functional;

3.Performing semi-empirical calculations using MNDO, AM1 and PM3 methods;

4. Optimization of geometry, search for transient states using analytical gradients;

5.Calculation of the frequencies of stretching vibrations of IR and Raman spectra;

6. Calculation of molecular properties such as dipole moment, electrostatic potential, electron and spin density, population analysis according to Mulliken and Löwdin;

7. Possibility of modeling the influence of the solvent.

The program HyperChem is the most optimal for use in quantum chemical and molecular dynamics calculations of molecules. This program is suitable for novice users and learning quantum chemistry. Program has its own integrated windowed interface, which is focused on working in screen mode. In the menu, you can select the theory level and type of calculation, perform the calculation and analyze the results. Calculations can be performed by molecular mechanics methods, semiempirical methods, DFT, HF and MP2 methods. The calculation type includes fixed geometry calculations, geometry optimization, vibration frequency calculations, and transient search. Various molecular surfaces can be plotted in the analysis, including orbitals, electron and spin densities, and electrostatic potential. After calculating the frequencies, you can visualize the IR spectrum and animate the modes of normal vibrations. The program runs on Windows, LINUX, MacOS. Free trial available.

Programs designed for calculating periodic structures are not studied in the classroom.

In laboratory classes in quantum chemistry, students perform calculations of various molecular structures using the HyperChem program. Everyone gets their own individual tasks (4 different connections). Calculations are carried out first for diatomic homonuclear and heteronuclear molecules, then for more complex structures. The procedure for working with the HyperChem program is in the guidelines. Geometry optimization, calculation of the dipole moment, MO energy, analysis and classification of different types of MO, calculation of the potential curve for a given bond, determination of the dissociation energy, visualization of vibrational states are carried out. The program allows you to deepen and systematize the knowledge gained in the theoretical study of quantum chemistry.

Reference

1. Игнатов С.К. Квантово-химическое моделирование атомно-молекулярных процессов. - Нижний Новгород: ННГУ, 2019. - 94 с.

2. Квантово-химические расчеты в программе GAUSSIAN по курсу «Физика низкоразмерных структур». Таганрог: Изд-во ТТИ ЮФУ, 2012, 100 с.

3. http://www.chemistry-software.com/pdf/Hyperchem_full_manual.pdf