

One of the most important goals of theoretical chemistry is a development of new computational methods, which are capable to predict various properties of molecules. For instance, the knowledge of a dipole moment allows for an assessment of how strong two polar molecules will attract each other, while the polarizability value describes the susceptibility to the deformation of the given electronic density under influence of an electrostatic field. Although the basic equations of quantum mechanics are known for a long time, their application for large molecules requires that many approximations should be made because of limited computer capabilities. Therefore a constant work is performed in science to simplify the problem of properties' calculations, so that the resulting methods are applicable for molecules of large sizes. One of the potential possibilities, taken into account in scientific literature, is the partition of the molecule into smaller overlapping fragments, called the fragmentation method. This method has been so far mainly utilized for the calculation of the energy. Such a calculation consists of obtaining energies for fragments and summing them with the respective corrections of the doubled fragments. In the current project we propose the extension of this method for molecular properties with an aim to develop the approach which allows to calculate electron densities and so-called density susceptibilities based on the fragmentation model. The application of this model will yield fragments, which will be small enough to apply for them the existing advanced methods of quantum chemistry for properties, allowing us to obtain accurate values for required molecular properties. The proposed method will be utilized for an analysis of changes in molecular properties, resulting from the interaction with another molecule, which partially envelops the first molecule. Such complexes are ubiquitous in chemistry and biology, therefore a possibility to perform calculations and to make predictions of properties' changes for these systems is very important from both theoretical and practical points of view.