DESCRIPTION FOR THE GENERAL PUBLIC

In recent years one can observe a tremendous progress in theoretical description of intermolecular forces. To make any predictions of properties involving weak intermolecular interactions, one needs to know the interaction energy surface, i.e., the dependence of this energy on the geometry of the complex. Due to the increasing efficiency of the algorithms and availability of ever-increasing computer resources, it is possible to calculate interaction energy surfaces of weakly bonded molecular complexes containing a dozen or so atoms with an accuracy that 10-15 years ago was available only in single-point benchmark calculations. A general goal of our research is to study theoretical methods of description of small clusters with spectroscopic accuracy, i.e., to obtain surfaces with an accuracy sufficient to provide theoretical spectra that can be useful in interpretation of results of spectroscopic experiments. One can expect that such *ab initio* surfaces would be accurate also in other applications, like calculation of scattering or thermodynamic properties. Most of the interaction-energy surfaces developed up to date use an approximation that the molecules in the complex are rigid, since surfaces taking into account all degrees of freedom of a cluster are expensive to obtain and difficult to use in applications. However, it has been already proved that such assumption introduces uncertainties, sometimes significant, into theoretical description of the matter.

In the present study we plan to develop a new method of generation of reduced-dimensionality surfaces with efficiently included effects of the nonrigidity of the interacting molecules. To achieve this goal the interaction energies will be averaged over the internal vibrations of the molecules, but taking place in the complex. To calculate the interaction energy, the highest possible level of theory will be used. The resulting surfaces can be used in the same way as the rigid-monomer ones, but the calculated properties should be more reliable. The new method will be tested for several weakly bound systems, including the very important complex of two water molecules. The proposed research should increase quality of interaction energy surfaces and produce a new generation of reduced-dimensionality surfaces applicable in various fields of physics and chemistry. For instance, extremely accurate spectroscopic measurements sometimes need theoretical guidance which can be provided if very accurate potential energy surfaces are available. In addition, the *ab initio* calculations have no limitations characteristic of some spectroscopic experiments, where parts of the spectra are not available due to technical reasons. One should also mention that in the calculations we can relatively easy set the desired conditions, like temperature, while the same is not always so easy to control in the experimental setup. For example, we can simulate conditions specific to various parts of the universe and calculate properties important for astrophysics. Moreover, it has been recently demonstrated that the predictions based on the highest-quality surfaces, for instance, of some thermodynamic properties, can be in some cases more accurate than experimental studies.