For the general public

Our previous documented studies involved the series of molecular dynamic simulations of isolated aromatic molecular systems – benzene - and has left a number of unanswered questions. One of many additional questions was published by professor Dunitz'a who in his work from 2009, has studied the benzene crystal (protonated and deuterated) at different temperatures and has found the different temperature expansion of the crystal unit cells containing different isotopes of the same element (here a hydrogen and deuterium). These differences were explained by changes in the effective size of the isotopes. Dunitz postulated that around the temperature of 170K the deuterium in benzene crystal becomes larger than the hydrogen atom and which has far-reaching implications and may be the basis for explanation of the inverse kinetic isotope effect.

Thus based on advanced computer simulations, we would like to explain the experimentally observed effect, and go one steps forward to touch frustrating in this field for years, questions such as whether the effect can be economically computed and how efficiently determine the volume of atoms? What is the impact of quantum effects, as we are dealing with light atoms and quite low temperatures? What is the impact of isotopic substitution on the dynamics of carbon atoms in the aromatic ring? Is the effect be observed for the isolated molecules? What is the distribution of the population of each conformation of benzene ring in the crystalline phase - is it similar to that observed for the isolated system, or maybe not? But the most fundamental question is: what is the impact of the temperature on all these effects?

As the isotope effect is a basic concept in chemistry understanding this phenomenon is on general interest and as such may influence and stimulate many other research fields.