Towards the H/D isotope effect
Size of benzene vs perdeuterated benzene

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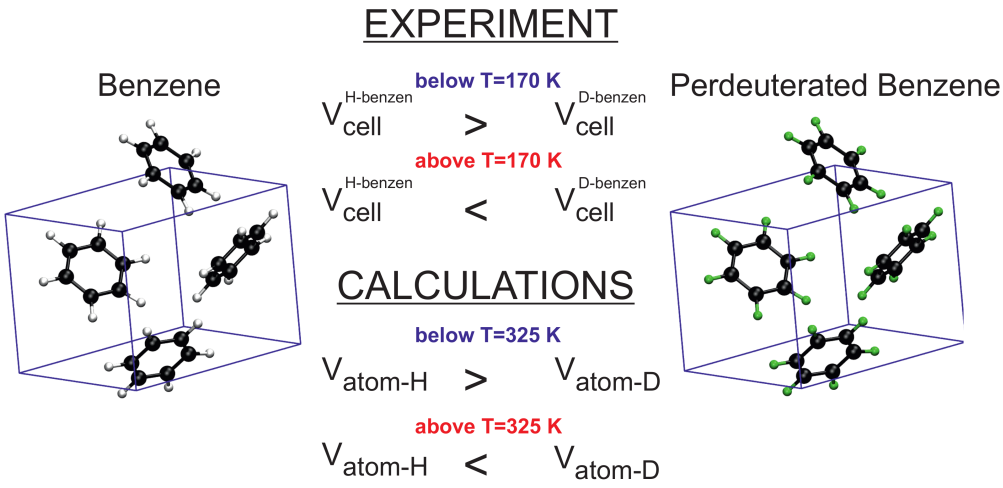
For crystalline systems isotope effect is manifested through different temperature expansion of unit cell volume of crystals containing distinct isotopes of the same element, as has been observed for benzene crystal and its perdeuterated counterpart. [1] The differences in temperature expansion of the cell are commonly attributed to changes of atomic effective sizes of isotopes due to atomic masses.

We propose to employ an innovative procedure [2] to determine the effective atomic sizes, based on three-steep routine in which the problem of finding an effective size of each atom is reduced to determination of volume inside which atom can be find with suitably high probability.

Our procedure is repeated for *ab initio* trajectories [3,4] computed with different target temperatures for benzene and perdeuterated benzene crystal and enables us to study temperature-driven changes of the effective size of H and D atoms.



References

1. J. D. Dunitz and R. M. Ibberson, *Angew. Chem. Int. Ed.* **47** (2008), 4208.
2. T. Duong, *J. Stat. Softw.* **21** (2008), 7.
3. R. Car and M. Parrinello *Phys. Rev. Lett.* **55** (1985), 2471.
4. D. Marx and J. Hutter *Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods*, Cambridge University Press, 2009.