Molecules in motion observed with x-rays

Klaus Braagaard Møller

Department of Chemistry, Technical University of Denmark, Kemitorvet 207, 2800 Kgs. Lyngby, Denmark
klaus.moller@kemi.dtu.dk

Progress in our understanding of ultrafast motion in molecules is best achieved through a close combination of experimental and theoretical approaches. Direct comparison is possible if theory is able to calculate experimental observables.

Ultrafast molecular motions are observed experimentally using pump-probe techniques where the processes of interest is initiated and monitored with ultrashort (femtosecond) flashes of electromagnetic radiation. This talk will first review some of our advances on the theory of femtosecond time-resolved x-ray scattering and prescriptions for calculating experimental observables [1,2].

Then, I will present combined experimental investigations and computer simulations of fundamental chemical processes of molecules in solution [3-8]. These involve bond formation [3-5], charge transfer [6-7] as well as intra- and intermolecular energy transfer and solvation dynamics. The experiments were carried out at the x-ray free-electron lasers LCLS (USA) and SACLA (Japan), and the computer simulations are multi-scale QM/MM molecular dynamics (MD) simulations.

Acknowledgments: DFF, Lundbeck Foundation, DanScatt, and my many collaborators.

References

[1] K.B. Møller and N.E. Henriksen, *Struct. Bond*. 2012, **142**, 185-212.
[2] A.O. Dohn, E. Biasin, K. Haldrup, M.M. Nielsen, N.E. Henriksen, and K.B. Møller, *J. Phys. B* 2015, **48**, 244010:1-8.
[3] J.H. Lee, M. Wulff, S. Bratos, J. Petersen, L. Guerin, J.-C. Leicknam, M. Cammarata, Q. Kong, J. Kim, K.B. Møller, and H. Ihee, *J. Am. Chem. Soc*. 2013, **135**, 3255-3261.
[4] A.O. Dohn, E.O. Jónsson, K.S. Kjær, T.B. van Driel, M.M. Nielsen, K.W. Jacobsen, N.E. Henriksen, and K.B. Møller, *J. Phys. Chem. Lett.* 2014, **5**, 2414-2418.
[5] T.B. van Driel, K.S. Kjær, R. Hartsock, A.O. Dohn, T. Harlang, M. Chollet, M. Christensen, W. Gawelda, N.E. Henriksen, J.G. Kim, K. Haldrup, K.H. Kim, H. Ihee, J. Kim, H. Lemke, Z. Sun, V. Sundstrom, W. Zhang, D. Zhu, K.B. Møller, M.M. Nielsen, and K.J. Gaffney *Nat. Commun.* 2016, accepted.
[6] S.E. Canton, K.S. Kjær, G. Vanko, T.B. van Driel, S. Adachi, A. Bordage, C. Bressler, P. Chabera, M. Christensen, A.O. Dohn, A. Galler, W. Gawelda, D. Gosztola, K. Haldrup, T. Harlang, Y. Liu, K.B. Møller, Z. Németh, S. Nozawa, M. Pápai, T. Sato, T. Sato, K. Suarez-Alcantara, T. Togashi, K. Tono, J. Uhlig, D.A. Vithanage, K. Wärnmark, M. Yabashi, J. Zhang, V. Sundström, and M.M. Nielsen, *Nat. Commun.* 2015, **6**, 6359:1-10.
[7] A.O. Dohn, K.S. Kjær, T. Harlang, S.E. Canton, M.M. Nielsen, and K.B. Møller, *Inorg. Chem.* 2016, accepted.
[8] E. Biasin, T.B. van Driel, K.S. Kjær, A.O. Dohn, M. Christensen, T. Harlang, P. Chabera, Y. Liu, J. Uhlig, M.I. Pápai, K.B. Møller, M.M. Nielsen, and K. Haldrup, *Phys. Rev. Lett.* 2016, **117**, 013002:1-6.