# CV and 10 year track record David van der Spoel

**Brief CV**

1. Ph. D. Biophysical Chemistry, 1996, University of Groningen, The Netherlands
2. Professor of Computational Molecular Biophysics 2008, Uppsala University
3. Chairman of the Board, Uppsala Multidisciplinary Centre for Advanced Computational Science (UPPMAX) from 2012-01-01.
4. 95 papers, 11800 citations and h-index 30.

**Top 10 publications 2002-present:**

**1.** C. Hetenyi & **D. van der Spoel**, Prot. Sci. 11 (2002) 1729-1737. 153 citations. Here we have introduced the so-called "Blind Docking" methodology, which has been adopted by hundreds of researchers world wide in academic environments as well as pharmaceutical companies. The method can be used to "scan" the surface of a bio-molecular receptor for possible (drug) binding sites, and yields a binding energy that can be validated by comparing to experimental data.

2. E.J.W. Wensink, A.C. Hoffmann, P.J. van Maaren and **D. van der Spoel**, J. Chem. Phys. **119** 7308-7317 (2003). 94 citations

3. **D. van der Spoel**, P. J. van Maaren, P. Larsson and N. Timneanu, J. Phys. Chem. B **110** pp. 4393-4398 (2006). 56 citations.

4. C. Caleman, P. J. van Maaren, M. Hong, J. S. Hub, L. T. Costa, **D. van der Spoel**, J. Chem. Theor. Comput. **8** pp. 61-74 (2012). 3 citations. These three papers (2-4) define our emphasis on industrial quality calculations of liquid properties. This work has culminated in the release to the public in 2011 of a web-server at http://virtualchemistry.org serving the broad scientific community within the field of physical chemistry.

5. M. Seibert, A. Patriksson, B. Hess and **D. van der Spoel**: J. Mol. Biol. **354** pp. 173-183 (2005), 79 citations.

6. **D. van der Spoel** and M. Seibert, Phys. Rev. Lett. **96** pp. 238102 (**2006**), 30 citations. In these two papers we demonstrated as the first group in the world that one can use computer simulations to follow the trajectory of a polypeptide from an extended chain into a folded conformation – and "predict" the structure of the peptide as determined experimentally *without using any experimental data to guide the process*. With this work we have in principle "solved" the protein folding problem.

7. **D. van der Spoel**, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J. C. Berendsen, J. Comp. Chem. **26** pp. 1701-1719 (2005), 1945 citations. I am the main architect of the GROMACS software (Groningen Machine for Chemical Simulation). At this point in time there are about 30 active developers over the world and thousands of users. The four main papers about the software have been cited more than 8600 times.

8. Patriksson, E. Marklund and **D. van der Spoe**l, Biochemistry **46** pp. 933-945 (2007), 48 citations. Biomolecules can be studied using mass spectrometry and a variety of other techniques *in vacuo*. There is a vivid community around these topics and a strong interaction between theoreticians like myself, and experimentalists. Our work has been pivotal to interpret mass spectrometry experiments in terms of protein conformations, and we have collaborated with groups in Sweden and at Harvard.

9. Caleman, J.S. Hub, P. J. van Maaren & **D. van der Spoel**, Proc. Natl. Acad. Sci. **108** (2011) 6838-6842, 19 citations. Related to the work on proteins in the gas phase are studies of evaporation from droplets and of ions in droplets. Here we have elucidated the energetic origin of surface solvation for halide anions, a result that has implications in atmospheric chemistry and climate modelling.

10. Larsson, Daniel S. D.; Liljas, Lars; **van der Spoel, David**, PLoS Comput. Biol. **8** (2012) e1002502, 1 citation. Some of the most ambitious biological simulations published to date, leading the way to deeper understanding of virus capsid morphology and to future drugs against capsid assembly.

**Invited presentations**

University of Bergen, Norway 2002, Stanford university, Stanford, USA, 2002, Symposium at the Manne Siegbahn laboratory, Stockholm, Sweden 2003, Annual meeting of the Swedish structural biology network, Tallberg, Sweden, 2003, First Canadian Workshop on Ultrafast Dynamic Imaging, Quebec, Canada 2003, X-FEL symposium, Himeji, Japan, 2004, IUCR meeting, Florence, Italy 2005, Para 06, Umeå, Swden, 2006, American Chemical Society Fall meeting, San Francisco USA, 2006, Industrial Fluid Properties Simulation Challenge workshop, St. Paul USA, 2006, Lawrence Livermore National Laboratories, Livermore, USA, 2006, Univ. California, San Francisco, USA, 2006, CCP workshop, Cambridge, UK, 2007, Tartu Univ., Estonia, 2007, GROMACS Workshop, CSC, Finland 2007, Computational Biomolecular summer school, Helsinki, Finland 2007, Oulu Univ. Finland, 2007, DESY, Hamburg, 2008, International Symposium of Post-graduation and Research (Sao Paolo, Brazil, 2008), Univ. Leiden, Netherlands, Mar 2009, Univ. Amsterdam, Netherlands, May 2009, DEISA Symposium, Amsterdam, May 2009, Hydrogen bonding conference Paris, Sept. 2009, IRB Barcelona, Nov. 2009, IBBI Berlin, June 2010, Fritz Haber Institute, Berlin, Oct. 2011, Novozymes, May 2011, CECAM meeting Dublin, May 2011, ACS Spring meeting, San Diego 2012, Eötvös Univ. Budapest, March 2012, ISQBP Meeting Stockholm 2012, Julich Bioscience 2012, Germany.

**Organization of International conferences**

I organized a workshop with 80 participants in 2008 in Uppsala in the context the use of X-ray free electron lasers for scattering experiments. Since my appointment as a post-doc at Uppsala University in 1997 I worked with Janos Hajdu on supporting the scientific case for building an experimental facility for photon science: the X-ray free electron laser. I performed computer simulations of a protein in an intense photon beam, the results of which were published in Nature (Neutze, Wouts, Van der Spoel, Weckert & Hajdu Nature 406 (2000) 752-757). This work was successful in the sense that funds - 100s of millions Euro respectively U.S. $ - to build such instruments were granted – one facility is operational in Stanford, and another under construction in Hamburg. Without this paper these facilities would most likely not have been funded.

**Major contributions to early careers of excellent researchers**

Two post-docs that worked under my supervision have both received grants to start their own group (Jochen Hub in Göttingen, Germany) and Carl Caleman (Uppsala University) following very productive periods (e.g. papers 4 and 9 above).

**Summary**

My work in the last ten years has laid the foundation for a huge international effort in photon science, we have demonstrated for the first time that it is tractable to solve the protein folding and structure prediction problem by computational means, we have introduced the blind docking methodology, we provided a structural description of proteins under mass spectrometry conditions, we develop the hugely popular simulation software GROMACS, and work on improved physical models for simulation, focusing particularly on liquids and liquid mixtures. Figure 1 shows citation data.

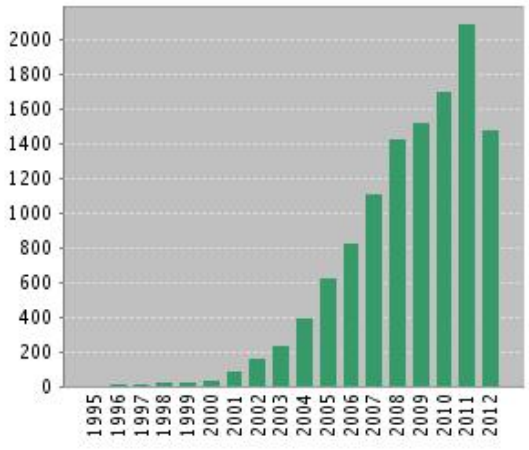


*Figure 1: Citations to D. van der Spoel from ISI Web of Knowledge*