Prof. Aatto LAAKSONEN, Senior Researcher

Positions: **2000-present**: **Professor**, (PhysChem, StatMech, Biophys., CompChem., Quantum Chemistry), Stockholm University (SU); **1984-present**: **PhD** supervisor, **20 PhD students** graduated; **1976-1999**: **Res. Ass., Ass. Prof., Senior Lecturer/Assoc. Prof.**, SU

Education: 1984: **Habilitation** Physical Chemistry**,** SU; **1981**: **PhD** Theoretical Chemistry, SU; **1976**: **MSc** Mathematics, SU

Editorial activity: member in the editorial board of Int. J. Quant. Chem., J. Comp. Theor. Nanosci

International conferences: 10+ in the organizing committee, **50+** as invited speaker

Research contracts: 20+ (10+ as project manager) (details in Section B3)

Expertise fields: Comp. Materials Sciences/Bio Sciences, Comp. Science, Theor. Spectroscopy

Evaluator for: Swedish, Irish, Israeli, Belgian & Romanian National Science Councils.

Fellowships: KAVLI fellow 2013 Beijing China. **STIAS** fellow 2014 Stellenbosch South Africa

Scientific results were published in more than **290 scientific papers** in international journals; 20+ books/ chapters books, **whose international impact/recognition in the field is reflected by**: **Hirsch factor** (WoS): **38**, Number of WoS independent citations > 4950, **Hirsch factor** (Google Scholar)**: 44**, Number of citations >7100.

Scientific achievements: One of the true pioneers in the Swedish computer simulations, he published the first studies in the field in late 70's. Since then, he coordinated a research group of **8-12 researchers** on three directions: molecular dynamics simulations of inter- and intramolecular NMR relaxation, simulation of nucleic acids, development of new computational methods.

In 90', ***long before coarse-graining and multi-scale modelling became mainstream***, he ***developed***: **i)** a *powerful method for coarse-graining, the Reverse Monte Carlo aproach*, to compute effective interaction potentials from radial distribution functions (A.P. Lyubartsev, **A. Laaksonen**, Phys. Rev. E, 52, 4, 3730-3737, 1995) – **405 independent citations** (346 in the last 10 years); **ii)** a *3D visualization scheme for solvation structures around (bio) molecules (*D. L. Bergman, L. Laaksonen, **A. Laaksonen**, J. Mol. Graph., 15, 5, 1997) – **349 independent citations** (245 in the last 10 years); **iii)** *a scalable portable parallel MD simulation package for arbitrary molecular mixtures* **(**A.P. Lyubartsev, **A. Laaksonen,** Comput. Phys. Commun., 128, 3, 565-589, 2000) – **246 independent citations** (203 in the last 10 years). Since then, he improved the simulation tools with QM/MM methods and coupling schemes, developed functional theory methods for large scale systems**,** expanded ensemble method to compute accurate absolute free energies and chemical potentials in a single Molecular Dynamics run (see Section B3.1). *Further, I was among the first that applied the above simulation tools on DNA, lipid bilayers, polymeric nanostructures***.** In 2012, Stockholm University identified **my research as "leading" in the area of "Biomodelling: from molecules to populations**".