Project leader (CO): Prof. Aatto LAAKSONEN

Professor in Physical Chemistry: 2000 - Stockholm University (SU);

1976 – 1999: Research Associate, Assistant Professor, Senior Lecturer/Associate Professor (SU)

Education: 1984: Habilitation Physical Chemistry, SU; **1976:** PhilCand Mathematics (major), SU; **1981:** PhD Theoretical Chemistry, SU

Post-doctoral stays: Daresbury Laboratory (UK) 1982, IBM laboratories (USA) Poughkeepsie 1983, Kingston 1984-85

Educator: 30+ years of teaching at all academic levels (General Chemistry, Physical Chemistry, Moleculer modelling), supervised 20 PhD students

Visiting Professor: Dalhousie University (Canada) 1993-94, Japan Atomic Energy Research Institute (Japan) 2002, 2005, University of Cagliari (Italy) 2008, 2009, 201, 2015, Nanyang Technological University (Singapore) 2017.

Senior Professor: Ångström Laboratory, Uppsala University 2018 - 2019

Distinguished Foreign Professor: Nanjing Tech University 2019 -

Project leader: iLEAP – Ionic liquids for lubrication 2014-2018

Project manager: EXSELENT center for porous materials 2007-2013

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**

Winter/Summer Schools & workshops (last 12 years as teacher): - School on Biological Soft Matter, São Paulo, Brazil 2017 - III Escola Brasileira de Modelagem Molecular 2015 - Molecular modeling, Kosice, Slovakia, 2015 - Advanced Molecular Simulation Methods in Physical Sciences Kavli Institute of Theoretical Physics, Beijing China, 2013 - II Escola Brasileira de Modelagem Molecular 2013 - Multi-scale modeling, Cagliari (2012), Namur, Belgium (2011), Changchun, China (2010), Singapore (2010) - CCP5 Summer school, Bath, UK (2006)

Expertise fields: Computational Materials Science, Biological Computations, Theoretical Spectroscopy, Multi-scale modelling.

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

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

Scientific achievements: Computer simulations of inter- and intramolecular NMR relaxation, simulation of canonical/non-canonical DNA, membrane proteins, anti-freeze proteins, modelling of zeolites, MOFs, ionic liquids, deep eutectic solvents, liquid crystals Development of numerous novel computational methods (QM/MM, inverse methods, tight-binding DFT, parallel algorithms, 3D visualisation etc). 300+ publications in international journals; 20+ book chapters, international impact/recognition in the field is reflected by: h-index (Google Scholar): 45, i10 index: 149, Number of citations >8000.