

Stefan Wallin

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ACADEMIC POSITIONS

- 2018 July 1 – (present) Assistant Professor (tenure track)
Department of Physics and Physical Oceanography, Memorial University
- 2015 Jul – 2018 Jun Assistant Professor (non-tenure track)
Department of Physics and Physical Oceanography, Memorial University
- 2008 Aug – 2015 Jun Assistant Professor (non-tenure track)
Department of Astronomy and Theoretical Physics, Lund University
- 2006 Jan – 2008 Jun Postdoctoral fellow
Department of Chemistry and Chemical Biology, Harvard University
- 2003 Oct – 2005 Dec Postdoctoral fellow
Department of Biochemistry, University of Toronto

EDUCATION AND DEGREES

- 2012 Docent in Theoretical Physics, Lund University
- 2003 Doctor of Philosophy in Theoretical Physics, Lund University
- 1999 Master of Science in Physics and Mathematics, Lund University

PUBLICATION RECORD

I have published **32** articles in international peer-reviewed journals (29 original research articles, 3 review articles), 1 conference proceeding and 1 book chapter, with a total of 1265 citations. My Hirsch index (h-index) is **18**. *Source:* Google Scholar.

RESEARCH GRANTS AND SCHOLARSHIPS

- 2020 – 2021 Computational resources grant, COMPUTE CANADA (Principal Applicant).
Title: Proteins in artificially crowded systems.
Total funding equivalent to \$6,916/year.
- 2020 – 2021 Teaching remission grant, Faculty of Science, Memorial (Principal Applicant).
Research-based competitive funding to reduce teaching load.
Total funding equivalent to \$5,000.
- 2017 – 2019 Computational resources grant, COMPUTE CANADA (Principal Applicant).
Fast-track renewed 2018 and 2019.
Title: The physics of conformational switching in proteins.
Total funding equivalent to \$9,442/year.

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| 2016 – 2021 | Research grant, NSERC Discovery (Principal applicant) Title: Computational studies of conformational switching in proteins Total funding: \$22,000/year for 5 years |
| 2015 – 2017 | Research grant, Start-up, Faculty of Science, Memorial (Principal applicant) Total funding: \$10,000/year for 2 years |
| 2010 | Research grant, Per-Eric and Ulla Schyberg foundation (Principal applicant) Title: Understanding and predicting protein-peptide interactions Two grants awarded among 50 applicants. Funding used to hire a postdoctoral fellow. Total funding: \$45,000 |
| 2008 – 2014 | Research grant, Swedish Research Council (Principal applicant) Title: Computer design and simulation of protein-peptide interactions Awarded for a non-tenure track assistant professor position at Lund University (in part for my salary). Total funding: \$693,000 |
| 2004 | Postdoctoral scholarship, Swedish Research Council (Principal applicant) For a two-year position at University of Toronto. Total funding: \$110,000 |
| 2004 | Postdoctoral scholarship, The Sweden-America Foundation, declined (Principal applicant) Total funding: \$8,000 |

OTHER FUNDING

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| 2017 | Conference grant, Memorial University Conference Fund (Co-applicant) Towards the organization of the international conference “Association in solution IV” hosted by Memorial July 30-Aug 4, 2017. Total funding: \$5,000 |
| 2011 | Conference grant, Nordic Institute for Theoretical Physics (Co-applicant) For the organization of a 3-week scientific workshop, Stockholm Total funding: \$30,000 |
| 2011 | Conference grant, Swedish Royal Physiographic Society (Co-applicant) For the organization of the 11th Swedish Bioinformatics Workshop, Lund Total funding: \$8,000 |
| 2011 | Conference grant, Gunnar and Gunnel Källén memorial fund (Co-applicant) For a “chalk-talk” series in computational biology (graduate students run) Total funding: \$15,000 |
| 2005 | Travel award, Canadian Institute of Health Research (Principal applicant) Total funding: \$ 1,500 |

SERVICE TO THE UNIVERSITY

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| 2020 | Selection committee, Terra Nova Young Investigator Award (Memorial) |
| 2020 | Hiring committee (department). 3-year teaching term position. |
| 2019 | Hiring committee (department). 3-year teaching term position. |
| 2018 – (present) | Graduate studies committee (departmental) |
| 2017 – 2019 | Adjudication committee, salary-based research grants (Memorial) |
| 2017 | Adjudication committee, Vitamin Research Fund (Memorial). 9 applications evaluated. Total funds available: \$700,000. |
| 2015 – 2018 | Undergraduate studies committee (department level) |
| 2015 – 2017 | Seminar committee (department level) |
| 2013 – 2015 | BSc thesis projects coordinator, BSc program in Theoretical Physics (Lund) |
| 2013 – 2015 | Study advisor (undergraduate), BSc program in Theoretical Physics (Lund) |
| 2012 – 2014 | Board member, LUNARC supercomputing facility (Lund). |

SERVICE TO THE FIELD

I review manuscripts for various international journals, including: *Journal of Chemical Physics*, *Journal of Physical Chemistry Letters*, *Physical Review E*, *Physical Review Letters*, *Biomembranes*, *Proteins*, *PLOS Computational Biology*, *Current Opinion in Structural Biology*, *Scientific Reports*. I reviewed proposals for the Breakout Labs program of the Thiel Foundation (California), which provides funding for early-stage tech companies.

List of journal article reviews while at Memorial (2015 Aug-present):

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| Jun 2020 | Proteins |
| Jul 2019 | Proteins |
| Jul 2019 | Physical Review E |
| Jul 2018 | Biophysical Journal |
| May 2018 | Proteins |
| Aug 2017 | Physical Review Letters |
| May 2017 | Physical Review Letters |
| Jun 2016 | Physical Review Letters |
| Aug 2016 | Current Opinion in Structural Biology |
| Oct 2015 | Scientific Reports |
| Sep 2015 | Journal of Physical Chemistry Letters |

Refereeing of research grants:

Jan 2020 NSERC Discovery Grant, external reviewer
Jan 2019 NSERC Discovery Grant, external reviewer

PRESENTATIONS

Invited talks at conferences and workshops:

2020 May Biophysical Society Canada Annual Meeting (invited). *Meeting postponed to 2021.*
2019 Jun CAP Annual Congress (contributed), Division of Physics in Medicine and Biology, Vancouver
2018 Oct CECAM workshop Peptide–Protein Interactions, Paris
2018 Jun Soft Matter Canada (workshop), Dalhousie University
2016 Jun CAP Annual Congress (invited), Division of Physics in Medicine and Biology, Ottawa
2014 Jun Pufendorf Institute symposium, Lund.
2012 May Center for Molecular Protein Science Symposium, Lund.
2009 Aug Kavli Institute for Theoretical Physics China (KITPC) conference, Chinese Academy of Sciences, Beijing, China.
2008 Sep International Centre for Theoretical Physics (ICTP) conference, Trieste, Italy.
2005 Apr 4th Annual Chemical Biophysics Symposium, Toronto.

Invited talks at universities:

2015 Nov Department of Physics and Atmospheric Science, Dalhousie University.
2015 Feb Department of Chemistry, University of Oklahoma, USA.
2014 Apr Department of Theoretical Chemistry, Lund University.
2013 Aug Department of Chemistry, Lund University.
2012 Dec Sainsbury Laboratory, Cambridge University.
2009 Apr Department of Chemistry, Cambridge University.

Poster presentations:

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| 2019 Mar | Annual Meeting of the Biophysical Society, Baltimore, US |
| 2018 Jun | CAP Annual Congress (Physics in Medicine and Biology Division), Halifax |
| 2010 Oct | IRB conference, Barcelona, Spain (poster) |
| 2007 Jul | 21th annual symposium of The Protein Society, Boston (poster) |
| 2005 Mar | Johns Hopkins Folding Meeting, St. Michaels, Delaware (poster) |
| 2005 Jun | ICTP workshop, Trieste, Italy (poster and talk) |
| 2004 Aug | Annual symposium of The Protein Society, San Diego, US (poster). |

TRAINING OF HIGHLY QUALIFIED PERSONNEL

* = principal supervisor

Postdocs:

| Name | University | Date |
|----------------------|------------|---------------------|
| Arnab Bhattacharjee* | Lund Univ | 2011 Mar – 2013 Feb |

Arnab is now an Assistant professor at Jawaharlal Nehru University, New Delhi, India.

Graduate students:

| Name | Program | University | Date |
|------------------------|---------|------------|----------------------|
| Saman Bazmi* | PhD | Memorial | 2019 Aug – (present) |
| Bahman Seifi* | PhD | Memorial | 2019 May – (present) |
| Aidan Tremblett* | MSc | Memorial | 2017 Sep – 2019 Aug |
| Adekunle Aina* | MSc | Memorial | 2016 Sep – 2018 Aug |
| Emil Ljungberg | MSc | Lund | 2013 Sep – 2014 Jan |
| Emelie Flood | MSc | Lund | 2013 Jan – 2014 Jan |
| Christian Holzgräfe* | PhD | Lund | 2010 Sep – 2014 Aug |
| Sigurdur Aegir Jonsson | PhD | Lund | 2009 Sep – 2014 Feb |
| Iskra Staneva* | PhD | Lund | 2008 Sep – 2012 Jun |
| Maja Klevanski | MSc | Harvard | 2007 Sep – 2008 Mar |

BSc honors theses:

| Name | Program | University | Date |
|---------------------|---------|------------|----------------------|
| Erica Short* | BSc | Memorial | 2020 Sep – (present) |
| Nicholas Robichaud* | BSc | Memorial | 2018 Sep – 2019 May |
| Daniel Trotter* | BSc | Memorial | 2017 Sep – 2018 May |
| Ryan Wilkins* | BSc | Memorial | 2015 Sep – 2016 May |
| Karolina Mothander* | BSc | Lund | 2015 Jan – Jun |
| Frieder Henning* | BSc | Lund | 2014 Sep – 2015 Jan |
| Daniel Nilsson* | BSc | Lund | 2014 Jan – Jun |
| Niels Linnemann* | BSc | Lund | 2012 Jan – Jun |

Other undergraduate training:

| Name | Program | University | Date |
|---------------------|----------------|-------------------|---------------------|
| Erica Short* | CSJ | Memorial | 2020 Jul – Sep |
| Nicholas Robichaud* | Summer | Memorial | 2019 May – Jul |
| Nicholas Robichaud* | USRA | Memorial | 2018 Jun – Aug |
| Victoria Trotter* | SURA | Memorial | 2017 Jun – Aug |
| Peter Gysbers* | work term | Memorial | 2015 May – 2016 Aug |
| Liam J Long* | MUCEP | Memorial | 2016 Nov – Dec |

TEACHING EXPERIENCE

Undergraduate level (F=Fall, W=Winter):

| Course | Name | Semester | Year | Role | University | Enrolment |
|---------------|-------------------------|-----------------|-------------|---------------------------|-------------------|------------------|
| PHYS 3400 | Thermal Physics | 2021 W | 3rd | Course leader | Memorial | TBD |
| PHYS 4400 | Statistical Mechanics | 2021 W | 4th | Course leader | Memorial | TBD |
| PHYS 3050 | Intro to Biophysics | 2020 W | 3rd | Course leader | Memorial | 6 |
| PHYS 4400 | Statistical Mechanics | 2020 W | 4th | Course leader | Memorial | 3 |
| PHYS 1021 | Introductory Physics II | 2019 F | 1st | Course leader | Memorial | 51 |
| PHYS 3050 | Intro to Biophysics | 2019 W | 3rd | Course leader | Memorial | 7 |
| PHYS 4400 | Statistical Mechanics | 2019 W | 4th | Course leader | Memorial | 5 |
| PHYS 1021 | Introductory Physics II | 2018 F | 1st | Course leader | Memorial | 51 |
| PHYS 4400 | Statistical Mechanics | 2018 W | 4th | Course leader | Memorial | 5 |
| PHYS 1021 | Introductory Physics II | 2018 W | 1st | Course leader | Memorial | 70 |
| PHYS 4400 | Statistical Mechanics | 2017 W | 4th | Course leader | Memorial | 5 |
| PHYS 1021 | Introductory Physics II | 2017 W | 1st | Course leader | Memorial | 112 |
| PHYS 3400 | Thermal Physics | 2016 F | 3rd | Course leader | Memorial | 12 |
| PHYS 4400 | Statistical Mechanics | 2016 W | 4th | Course leader | Memorial | 2 |
| PHYS 3400 | Thermodynamics | 2015 F | 3rd | Course leader | Memorial | 13 |
| FYTK01 | BSc Degree Project | 2015 W | 4th | Course leader | Lund | 8 |
| FYTN05 | Theoretical Biophysics | 2014 F | 3rd | Course leader | Lund | 19 |
| FYTK01 | BSc Degree Project | 2014 W | 4th | Course leader | Lund | 9 |
| FYTN05 | Theoretical Biophysics | 2013 F | 3rd | Course leader | Lund | 13 |
| FYTN05 | Theoretical Biophysics | 2012 F | 3rd | Course leader | Lund | 21 |
| FYTN05 | Theoretical Biophysics | 2011 F | 3rd | Course leader | Lund | 16 |
| FYTN05 | Theoretical Biophysics | 2010 F | 3rd | Course leader | Lund | ≈15-20 |
| FYTN05 | Theoretical Biophysics | 2009 F | 3rd | Course leader | Lund | ≈15-20 |
| PHYSICI 1 | Physical Sciences 1 | 2007 W | 1st | TA/problem session leader | Harvard | ≈25 |

Graduate-level:

| Course Name | Semester | Role | University | Delivery mode | Enrolment |
|--------------------------------------|----------------|----------------|---------------------|-----------------------|-----------|
| PHYS 6400 Statistical Mechanics | 2021 W | Course leader | Memorial | Seminars+ Lectures | TBD |
| PHYS 6040 Biophysics | 2020 W | Course leader | Memorial | Seminars+ Lectures | 5 |
| PHYS 6040 Biophysics | 2019 W | Course leader | Memorial | Seminars+ Lectures | 4 |
| PHYS 6413 Soft Matter | 2017 F | Guest lecturer | Memorial | Lectures | ≈5-10 |
| Grad course in Protein Physics | 2011 W | Course leader | Lund | Seminars | 8 |
| Grad course in Physical Chemistry | 2010-11 F+W | Guest lecturer | Lund (Chemistry) | Lectures | ≈10 |

In 2000-2003, I held teaching assistantships, including problem session leader and laboratory teaching assistant, in various undergraduate physics courses at Lund University.

RECOGNITIONS

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| 2019 Nov | “Editor’s Suggestion” feature of article Nicholas Robichaud, Ivan Saika-Voivod and Stefan Wallin, <i>Physical Review E</i> 100 052404 (2019). |
| 2018 Nov | Featured in CAP Newsletter, Division of Physics in Medicine and Biology. |
| 2014 Sep | “New and Notable” feature of article Christian Holzgräfe and Stefan Wallin, <i>Biophysical Journal</i> 107 1217 (2014): Robert Best, “Bootstrapping new protein folds”, <i>Biophysical Journal</i> 107 1040-1041 (2014). |
| 2010 Apr | Award, Per-Eric and Ulla Schyberg foundation, for research on protein-peptide interactions |

EVENT ORGANIZATION

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|--------------|---|
| 2017 Jul-Aug | Local co-organizer, international conference “Association in Solution IV”, Memorial University |
| 2012 Feb-Mar | Co-organizer, 3-week NORDITA scientific program “Dynamics of biomolecular processes: from atomistic representations to coarse-grained models,” Stockholm. |
| 2011 Sep | Co-organizer, 11th Swedish Bioinformatics Workshop “Systems biology and comparative genomics”, Lund University. |

OUTREACH ACTIVITIES

Popular science talks given:

| Date | Title of talk | Venue | Audience |
|-------------|---|--------------|----------------------|
| 2013 Mar | Proteiner löser trassliga problem: om knutar i biomolekyler (Proteins solve entangled problems: on knots in biomolecules) | Lund | High school students |
| 2012 Sep | Från det minsta till det största, och det viktigaste däremellan: Hur kan så mycket viktigt få plats i en cell? (From smallest to largest: How do so many things fit in a cell?) | Lund | General public |
| 2011 Mar | Proteiner löser trassliga problem: om knutar i biomolekyler (Proteins solve entangled problems: on knots in biomolecules) | Lund | High school students |
| 2010 Sep | Proteiner löser trassliga problem: om knutar i biomolekyler (Proteins solve entangled problems: on knots in biomolecules) | Lund | General public |
| 2010 Mar | Knutar och annat trassel i bio-molekyler (Knots and other entanglements in biomolecules) | Lund | High school students |
| 2009 Mar | Knutar och annat trassel i bio-molekyler (Knots and other entanglements in biomolecules) | Lund | High school students |

Organization:

2014-2015 Coordinator, biannual popular science lecture series (Natur- och teknikvetarcirkeln) aimed at the general public and supported jointly by Lund University & Folkuniversitetet. I developed series themes, contacted speakers, and publicized events.

PUBLICATIONS

author name **in bold** = student under my supervision
[n] = number of citations (Source: Google Scholar)

Submitted manuscripts:

1. **B Seifi** and S Wallin. The C-terminal domain of transcription factor RaH: Folding, fold switching and energy landscape. In special issue “Fold-Switching Proteins” in *Biopolymers* (under review).

Articles and accepted manuscripts in peer-reviewed journals:

2. **B Seifi**, **A Aina** and S Wallin (2020). Structural fluctuations and mechanical stabilities of the metamorphic protein RfaH. *Proteins: structure, function and bioinformatics* (accepted).
3. **D Trotter** and S Wallin (2020). Effects of topology and sequence in protein folding linked via conformational fluctuations. *Biophysical Journal* **118** 1370–1380.
4. **N A Robichaud**, I Saika-Voivod and S Wallin (2019). Phase behavior of “blocky” charge lattice polymers: Crystals, liquids, sheets, filaments and clusters. *Physical Review E* **100** 052404. [3] **Editor’s Suggestion**
5. B M Coady, J D Marshall, L E Hattie, A E Brannan, M N Fitzpatrick, K E Hickey, S Wallin, V Booth and R J Brown (2018). Characterization of a peptide containing the major heparin binding domain of human hepatic lipase. *Journal of Peptide Science* **24** e3123.
6. **A Aina** and S Wallin (2017). Multisequence algorithm for coarse-grained biomolecular simulations: exploring the sequence-structure relationship of proteins. *Journal of Chemical Physics* **147** 095102. [2]
7. L Zhu, J Petrova, **P Gysbers**, H Hebert, S Wallin, C Jegerschöld and J. O. Lagerstedt (2017). Structures of Apolipoprotein A-I in High Density Lipoprotein generated by Electron Microscopy and Biased Simulations. *Biochimica et Biophysica Acta (BBA)-General Subjects* **1861** 2726-2738. [6]
8. S Wallin (2017). Intrinsically disordered proteins: structural and functional dynamics. *Research and Reports in Biology* **8**, 7-16. [8]
9. **C Holzgräfe** and S Wallin (2015). Local versus global fold switching in protein evolution: insight from a continuous 3-letter model. *Physical Biology* **12**, 026002 [4]
10. **C Holzgräfe** and S Wallin (2014). Smooth functional transition across a mutational pathway with an abrupt protein fold switch. *Biophysical Journal* **107**, 1217-1225 [17]
11. J Petrova, **A Bhattacharjee**, W Boomsma, S Wallin, J O Lagerstedt and A Irbäck (2014). Conformational and aggregation properties of the 1-93 fragment of apolipoprotein A-I. *Protein Science* **23**, 1559-1571 [11]
12. **A Bhattacharjee** and S Wallin (2013). Exploring protein-peptide binding specificity through computational peptide screening. *PLOS Computational Biology* **9**, e1003277 [23]
13. E Follin, M Karlsson, C Lundegaard, M Nielsen, S Wallin, K Paulsson and H Westerdahl (2013). In silico peptide-binding predictions of passerine MHC class I reveal similarities across distantly related species, suggesting convergence on the level of protein function. *Immunogenetics* **65**, 299-311 [11]

14. A Irbäck, S Ægir Jónsson, **N Linnemann**, B Linse and S Wallin (2013). Aggregate geometry in amyloid fibril nucleation. *Physical Review Letters* **110**, 058101 [45]
15. N Olsson, S Wallin, P James, C A K Borrebaeck and C Wingren (2012). Epitope-specificity of recombinant antibodies reveals promiscuous peptide-binding properties. *Protein Science* **21**, 1897-1910 [31] Cover feature
16. **I Staneva**, Y Huang, Z Liu and S Wallin (2012). Binding of two intrinsically disordered peptides to a multi-specific protein: A combined Monte Carlo and molecular dynamics study. *PLOS Computational Biology* **8**, e1002682 [46]
17. **A Bhattacharjee** and S Wallin (2012). Coupled folding-binding in a hydrophobic/polar protein model: Impact of synergistic folding and disordered flanks. *Biophysical Journal* **102**, 569-578 [37]
18. **I Staneva** and S Wallin (2011). Binding free energy landscape of domain-peptide interactions. *PLoS Computational Biology* **7**, e1002131 [18]
19. H S Chan, Z Zhang, S Wallin and Z Liu (2011). Cooperativity, non-local coupling, and nonnative interactions: Principles of protein folding from coarse-grained models. *Annual Review of Physical Chemistry* **62**, 301-326 [148]
20. **I Staneva** and S Wallin (2009). All-atom Monte Carlo approach to protein-peptide binding. *Journal of Molecular Biology* **393**, 1118-1128 [21]
21. A Zarrine-Afsar, S Wallin (co-first author), A M Neculai, P Neudecker, P L Howell, A R Davidson and H S Chan (2008). Theoretical and experimental demonstration of the importance of specific nonnative interactions in protein folding. *Proceedings of the National Academy of Sciences USA* **105**, 9999-10004 [122]
22. J S Yang, S Wallin (co-first author) and E I Shakhnovich (2008). Universality and diversity of folding mechanics for three-helix bundle proteins. *Proceedings of the National Academy of Sciences USA* **105**, 895-890 [78]
23. S Wallin and E I Shakhnovich (2008). Understanding ensemble protein folding at atomic detail. *Journal of Physics: Condensed Matter* **20**, 283101 [13]
24. S. Wallin, K B Zeldovich and E I. Shakhnovich (2007). Folding mechanics of a knotted protein. *Journal of Molecular Biology* **368**, 884-893 [135]
25. S Wallin and H S Chan (2006). Conformational entropic barriers in topology-dependent protein folding: Perspectives from a simple native-centric polymer model. *Journal of Physics: Condensed Matter* **18**, S307-S328 [48]
26. S Wallin and H S Chan (2005). A critical assessment of the topomer search model of protein folding using a continuum explicit-chain model with extensive conformational sampling. *Protein Science* **14**, 1643-1660 [38]
27. G Favrin, A Irbäck and S Wallin (2003). Sequence-based study of two related proteins with different folding behaviors. *Proteins: Structure, Function, and Bioinformatics* **54**, 8-12 [4]
28. S Wallin, J Farwer and U Bastolla (2003). Testing similarity measures with continuous and discrete protein models. *Proteins: Structure, Function, and Genetics* **50**, 144-157 [47]
29. A Irbäck, B Samuelsson, F Sjunnesson and S Wallin (2003). Thermodynamics of alpha- and beta-structure formation in proteins. *Biophysical Journal* **85**, 1466-1473 [74]
30. G Favrin, A Irbäck, B Samuelsson and S Wallin (2003) Two-state folding over a weak free-energy

barrier. *Biophysical Journal* **85**, 1457-1465 [14]

31. G Favrin, A Irbäck and S Wallin (2002). Folding of a small helical protein using hydrogen bonds and hydrophobicity forces. *Proteins: Structure, Function, and Genetics* **47**, 99-105 [84]
32. A Irbäck, F Sjunnesson and S Wallin (2000). Three-helix-bundle protein in a Ramachandran model. *Proceedings of the National Academy of Sciences USA* **97**, 13614-13618 [116]

Peer-reviewed conference proceedings and book chapters:

33. S Wallin (2017). Binding specificity profiles from computational peptide screening. In Ora Schueler-Furman and Nir London (eds.) "Modeling peptide-protein interactions: Methods and Protocols", *Methods in Molecular Biology* **1561**, Springer Press. [1]
34. A Irbäck, F Sjunnesson and S Wallin (2001). Hydrogen bonds, hydrophobicity forces and the character of the collapse transition. In P Bruscolini et al. (eds), Proceedings of the ISI Workshop "Protein Folding: Simple Models and Experiments", *Journal of Biological Physics* **27**, 169-179. [26]

Other published works:

34. H Behringer, R Eichhorn and S Wallin (2013). Dynamics of biomolecular processes. *Physica Scripta* **87**, 058501