# Dr. Giovanni Settanni

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*Theoretical and computational studies of biomolecule dynamics, assembly and adsorption*

## Personal

**Birth:** March 1, 1973, Triggiano (BA), Italy
**Nationality:** Italian

## Education

**1997 - 2001** **PhD,** Condensed Matter Theory Sector, SISSA, Trieste, Italy Thesis: "The role of native state topology in protein folding and dynamics". supervisors Prof. Amos Maritan and Prof. Paolo Carloni. Approved *cum laude*.

**1997 - 1998** **Master,** Condensed Matter Theory Sector, SISSA, Trieste, Italy Thesis: "Potential extraction by threading", supervisor Prof. Amos Maritan. Full marks.

**1992 - 1997** **Degree in Physics (Laurea in Fisica),** University of Turin, Italy. Thesis: "Aspects of learning in realistic neural networks", supervisor Dr. Alessandro Treves (SISSA, Trieste). Full marks *cum laude* and *menzione d'onore (average score on exams higher than 99%*).

## Academic Appointments

**2010 - present** **Group leader,** Physics Department, J. Gutenberg University, Mainz, Germany. Research activity: Theoretical and Computational Biophysics.

**2014 - 2021** **Scientific Coordinator,** Collaborative Research Center 146, J. Gutenberg University, Mainz, Germany

**2010 - 2019** **Junior faculty,** Max-Plank Graduate Center and Physics Department, J. Gutenberg University, Mainz, Germany.

**2005 - 2010** **Postdoctoral scientist** in Prof. Fersht's Lab**,** MRC Centre for Protein Engineering, Cambridge, UK. Research activity: Theoretical Biophysics and Molecular Dynamics Simulations for the Characterization of the Folding Process of Proteins and Peptides.

**2001 - 2004** **Postdoctoral research assistant** in Prof. Caflisch's Group, Biochemisches Institut, University of Zurich, Switzerland. Research activity: Folding Transition State of Proteins and Peptides investigated by Molecular Dynamics Simulations.

**1997** **Research contract,** Cognitive Neuroscience Sector, SISSA, Trieste, Italy. Project: "Aspects of learning in realistic neural networks".

## ***Grants, Awards & Qualifications***

**2021** High performance computing center Stuttgart, project no. ACID 44059 "Nanoparticle-biomolecule interactions investigated using molecular dynamics simulations", 10.0 millions core hours.

**2016** High performance computing center Stuttgart, project no. ACID 44059 "Adsorption properties of blood proteins investigated by molecular dynamics simulations", 30.8 millions core hours.

**2015** High performance computing center Stuttgart, project no. ACID 44059 "Fibrinogen flexibility and adsorption properties investigated by molecular dynamics simulations",11.5 millions core hours.

**2014** Italian national academic qualification as associate professor (Abilitazione Scientifica Nazionale Professore II Fascia) Sector 05/E1 General and Clinical Biochemistry

**2013** Italian national academic qualification as associate professor (Abilitazione Scientifica Nazionale Professore II Fascia) Sector 02/B2 Theoretical Condensed Matter Physics

**2012** Juelich Supercomputing Centre, project HMZ29, "Computer simulations of Fibrinogen adsorption on material surfaces", 90000 Node-hours

**2009** MRC-Centre for Protein Engineering Additional Salary Reward.

**2008** Poster presentation award at Gordon Research Conference on Protein Folding Dynamics, Ventura, CA, USA

**2006** Swiss National Science Foundation Young Scientist Fellowship (~12'000 GBP).

**2005** Stiefel-Zangger Stiftung fellowship (~24'000 GBP).
Novartis Foundation research support (~6'000 GBP).
EMBO Short term fellowship (~4'500 GBP).

**2002** IUPAB Travel Fellow Award to attend the IUPAB meeting, Buenos Aires, Argentina.

**2001** Grant for the FEBS Meeting, Lisbon, Portugal.

**2000** Grant for the Varenna School of Physics, Varenna, Italy.

**1998** Grant for the NATO ASI Soft Condensed Matter Conference, Geilo, Norway.

**1997** - PhD fellowship at SISSA, Trieste, Italy, Condensed Matter Theory Sector
- PhD fellowship at SISSA, Trieste, Italy, Neuroscience Sector (declined)
- Grant for the School on Vectorial and Parallel Computing, CINECA, Bologna, Italy.

**1993** Academic excellence award, University of Turin, Turin, Italy.

**1992** Selected for the final stage of the Italian Mathematics Olympic Games, Cesena, Italy.

**1991** 1st rank (regional), 3rd rank (national) at the Italian Chemistry Games (*Lyceum* category), Turin and Frascati, Italy.

## ***Teaching Activity***

**2011 – present** **Johannes Gutenberg Univerity, Mainz, Germany**
Teaching courses in Physics:
"Soft Matter Theory",
"Computer simulations in Statistical Physics",
"Advanced Simulation Methods",
"Modern computational methods in condensed/soft matter physics"
Teaching courses in Computer Science:
"Structural Bioinformatics"

**2011 – present** **Johannes Gutenberg Univerity, Mainz, Germany**
Co-Supervision of graduate, master and bachelor students (see below for list of thesis).

**2005 – 2011** **MRC-Centre of Protein Engineering, Cambridge, UK**
Co-Supervision of a graduate student on the research project: "Protein folding transition state investigated by Molecular Dynamics simulations"

**2002 – 2004** **University of Zurich, Biochemistry Department**
Co-supervision of graduate students on projects related to Molecular Dynamics Simulations of biological systems

**1998 – 2000** **SISSA Trieste, Italy**
Tutor of undergraduate students of the University of Trieste on Mathematics

## List of supervised Thesis

**Isolde H. Radford, PhD** "Implicit-Solvent Molecular Dynamics Simulations of Peptide Folding" (2011), University of Cambridge, UK, in collaboration with Prof. Alan Fersht

**Federico Amadei, Master** "Linking force and catalysis via PR65, the HEAT scaffold subunit of phosphatase PP2A" (2014), Ecole Normale Superieure de Lyon, Université de Lyon 1, France

**Lorenz Ripka, Master** "Molecular Dynamic Simulations of Fibrinogen-Complex Using Enhanced Sampling Techniques" (2014), University of Mainz, Germany

**Timo Schäfer, Bachelor,** "Influence of FlAsH-binding on the mechanical unfolding of the scaffold subunit of phosphatase PP2A" (2015), University of Mainz, Germany

**Stephan Köhler, PhD** "Modelling and simulation of fibrinogen and its adsorption behavior"(2015), University of Mainz, Germany, in collaboration with Prof. Friederike Schmid

**Florian Thomas, Bachelor** "Improving the efficiency of clustering algorithms for biomolecular simulations using GPUs"(2016), University of Mainz, Germany

**Timo Schäfer, Master,** "Metadynamics simulations of the fibrinogen protomer" (2017), University of Mainz, Germany, in collaboration with Prof. Friederike Schmid

**Thomas Kolbe, Bachelor,** "Deep Autoencoder for the Analysis of Molecular Dynamics Trajectories" (2020), University of Mainz, Germany

**David Noel Zimmer, Bachelor,** "Mulitscale Modeling of Lipid Nanoparticles" (2020), University of Mainz, Germany

## ***Organization of schools/workshops:***

IRTG school, Oct. 2015, Johannes Gutenberg University Mainz, Germany
CECAM school "Multiscale simulations of soft matter with VOTCA and ESPRESSO++ tutorial", Oct. 10-13 2016, Schloss Waldthausen, Mainz, Germany
CECAM school "Multiscale simulations of soft matter", Sep. 26-29 2017 Fulda, Germany
CECAM/CSM/IRTG school "Machine Learning in Scientific Computing", Sep. 10-14 2018 Nierstein, Germany
CECAM/IRTG school "Bio/Soft Matter Simulations across Multiple Scales", Sep. 18-20 2019 Heidelberg, Germany
IRTG school of the TRR146 2020, Dec. 02-04 2020 Virtual event via zoom
CECAM workshop "Mainz Materials Simulation Days 2021 - What Precision is Needed to Create Function: Roles of Defects and Disorder in Hierarchical Structure Formation of Soft Matter", Jun. 7-9 2021, Virtual event, Zoom/Discord

## ***Editorial and Reviewing work:***

Reviewing grant proposals submitted to:
European Research Council (Marie Curie Fellowships),
The American Chemical Society Petroleum Research Fund,
Engineering and Physical Sciences Research Council (EPSRC) UK,
British Council BIRAX,
EEA Grants - collaborative research projects - Norway Grants, UEFISCDI, Romania.

Reviewing manuscripts submitted to:
Proc. Natl. Acad. Scie. USA,
ACS Nano,
npj Computational Materials,
eLife,
PLOS Computational Biology,
Langmuir,
Biochemistry,
Physical Chemistry Chemical Physics,
Organic & Biomolecular Chemistry,
Journal of Physical Chemistry,
Journal of Chemical Physics,
Journal of Chemical Theory and Computation,
Organic and Biomolecular Chemistry,
European Biophysics Journal,
Biointerphases,
Journal of Molecular Liquids,
Molecular Systems Design & Engineering,
Biophysical Chemistry,
Proteins: Structure, Function, and Bioinformatics,
BMC Structural Biology,
Adhesive and Adhesion.

## ***Languages and technical skills:***

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|---|---|
| Italian | Mother tongue |
| English | Fluent |
| German | Level B2 |
| UNIX operating systems, tools, scripting languages (bash, csh, tcsh, awk, perl, tcl) and Linux cluster management | Extensive experience |
| High performance computer environments (SLURM, PBS Pro, LSF, TORQUE/MOAB) | Extensive experience |
| Windows operating system and tools | Extensive experience |
| C, Fortran, Python programming | Extensive experience |
| Molecular dynamics and visualization packages: CHARMM, NAMD, GROMACS, AMBER, VMD, Pymol, Marvin Sketch, Avogadro | Extensive experience |
| Parallel programming (MPI and OpenMP) and GPU programming | Extensive experience |
| Machine and deep learning tools (Tensorflow, KERAS, scikit-learn) | Extensive experience |

## ***Other Activities***

**People management and supervision :**

- scientific coordination of the activities of the Collaborative Research Center 146 and its integrated training research group, 2014-2021;
- coordination of the students activities of the Max-Plank graduate Center, Mainz, 2011/12.

**Budget or resource management :**

- Budget of Junior Faculty member of Max-Plank Graduate Center.
- management of the budget devoted to the purchase of the computer facilities (computer cluster, data storage, backup systems etc. ~15'000GBP) needed for computational research at the Centre for protein engineering.

**IT Administrative duties** :

- Management of the SFB-TRR146 Webpage https://trr146.de, 2014-2021, Department of Physics, Uni Mainz.
- IT management of the computer cluster, 2005-2011, at the MRC-Centre for protein engineering, Cambridge.
- IT management of Linux workstations and sector web-pages, 1998-2001, SISSA, Trieste, Italy.

## ***List of Publications***

*(total citations 1669, h-index 20, source: Google Scholar 6.2021)*

### Articles in peer reviewed journals

Schäfer, T. M; **Settanni**, G.;
Data reweighting in metadynamics simulations,
*J Chem Theory Comput.* **2020** 16(4):2042-2052

Bauer, M R; Krämer, A; **Settanni**, G; Jones, R N; Ni, X; Khan Tareque, R; Fersht, A R; Spencer, J; Joerger, A C;
Targeting cavity-creating p53 Cancer mutations with small-molecule stabilizers: the Y220X paradigm
*ACS chem biol.* **2020**, 15(3):657-668

**Settanni**, G; Schäfer, T; Muhl, C; Barz, M; Schmid, F;
Poly-Sarcosine and Poly (ethylene-glycol) interactions with proteins investigated using molecular dynamics simulations
*Comput. Struct. Biotechnol J.* **2018** 16:543-550

**Settanni**, G; Zhou, J; Schmid, F;
Interactions between proteins and poly (ethylene-glycol) investigated using molecular dynamics simulations
J. Phys. Conf. Ser **2017** 921(1):12002

Tüting L., Ye W., **Settanni** G., Schmid F., Wolf B. A., Ahijado-Guzmán, Rubén and Sönnichsen, C.
Potassium Triggers a Reversible Specific Stiffness Transition of Polyethylene Glycol
*J Phys Chem C.* **2017**, 121(40):22396–22402

**Settanni** G, Zhou J, Suo T, Schöttler S, Landfester K, Schmid F, Mailänder V.
Protein corona composition of poly(ethylene glycol)- and poly(phosphoester)-coated nanoparticles correlates strongly with the amino acid composition of the protein surface.
*Nanoscale*. **2017**; 9(6):2138-2144

Köhler S., Schmid F., **Settanni G.**
Molecular Dynamics Simulations of the Initial Adsorption Stages of Fibrinogen on Mica and Graphite Surfaces.
*Langmuir*. **2015**; 31(48):13180-90

Köhler S., Schmid F., **Settanni G.**
The Internal Dynamics of Fibrinogen and Its Implications for Coagulation and Adsorption
*PLoS Comput Biol*. **2015**; 11(9):e1004346

**Settanni G.**, Serquera D., Marszalek P.E., Paci E., Itzhaki L.S.
Effects of ligand binding on the mechanical properties of ankyrin repeat protein gankyrin.
*PLoS Comput Biol*. **2013**;9(1):e1002864

Radford IH, Fersht AR, **Settanni G.**
Combination of Markov state models and kinetic networks for the analysis of molecular dynamics simulations of peptide folding.
*J Phys Chem B*. **2011** 115(22):7459-71

Wetzel S.K., Ewald C., Jurt S., **Settanni G.**, Plückthun A. And Zerbe O.
Residue-resolved stability of full-consensus ankyrin repeat proteins probed by NMR
*J. Mol. Biol.* **2010** 402(1):241-58

Serquera D., Lee W., **Settanni G.**, Paci E., Marszalek P.E. and Itzhaki L.S.
Mechanical unfolding of an ankyrin repeat protein
*Biophys. J.* **2010** 98(7):1294-301

Basse N., Kaar J. L., **Settanni G.**, Joerger A. C., Rutherford T. J., Fersht A. R.
Towards the Rational Design of p53 Stabilizing Drugs: Probing the Surface of the OncogenicY220C Mutant
*Chemistry & Biology*, **2010** 17(1):46-56

Huang F., Rajagopalan S., **Settanni G.**, Marsh R., Armoogum D., Nicolaou N., Bain A., Lener E., Haas E., Ying L., Fersht A. R.
Multiple conformations of full-length p53 detected with single-molecule fluorescence resonance energy transfer.
*Proc. Natl. Acad. Scie. USA*. **2009** 106(49):20758-20763

**Settanni G.**, Fersht A. R.
Downhill versus barrier-limited folding of BBL 3. Heterogeneity of the native state of the BBL peripheral subunit binding domain and its implications for folding mechanisms.
*J. Mol. Biol.* **2009** 387(4):993-1001

Yu G.W., Vaysburd M., Allen M.D., **Settanni G.** and Fersht A.R.
The structure of human MDM4 N-terminal domain bound to a single domain antibody
*J. Mol. Biol.* **2009** 385(5):1578-89

**Settanni G.**, Fersht A. R.
High Temperature Unfolding Simulations of the TRPZ1 peptide
*Biophys. J.* **2008** 94(11):4444-53

Huang F., **Settanni G.**, Fersht A. R.
Fluorescence resonance energy transfer analysis of the folding pathway of Engrailed Homeodomain. *Protein Eng. Des. Sel.* **2008** 21(3):131-46

Wetzel S.K., **Settanni G.**, Kenig M., Binz K., Plückthun A.
Folding and Unfolding Mechanism of Highly Stable Full Consensus Ankyrin Repeat Proteins
*J. Mol. Biol.* **2008** 376(1):241-57

Interlandi G., Wetzel S.K., **Settanni G.**, Plückthun A., Caflisch A.
Unfolding of designed ankyrin repeat proteins characterized by molecular dynamics simulations and chemical denaturation experiments
*J. Mol. Biol.* **2008** 375(3):837-54

Seeber M., Cecchini M., Rao F., **Settanni G.**, Caflisch A.
Wordom: a program for efficient analysis of molecular dynamics simulations
*Bioinformatics*. **2007** 23(19):2625-7

Interlandi G., **Settanni G**., Caflisch A.
Unfolding transition state and intermediates of the tumor suppressor p16INK4a investigated by molecular dynamics simulations.
*Proteins.* **2006** Jul 1;64(1):178-92.

Rao F., **Settanni G**., Guarnera E., Caflisch A.
Estimation of protein folding probability from equilibrium simulations.
*J. Chem. Phys.*, **2005**, 122:184901

**Settanni G**., Rao F., Caflisch A.
Phi-value analysis by molecular dynamics simulations of reversible folding
*Proc. Natl. Acad. Scie. USA,* **2005**, 102:628-33.

**Settanni G**., Gsponer J., Caflisch A.
Formation of the folding nucleus of an SH3 domain investigated by loosely coupled molecular dynamics simulations
*Biophys J.*, **2004**; 86:1691-1701

**Settanni G.**, Cattaneo, A., Carloni P.
Molecular Dynamics Simulations of the NGF / TrkA domain 5 Complex and Comparison with

Biological Data
*Biophys J.* **2003** Apr;84(4):2282-92.

**Settanni, G.**, Hoang, T.X., Micheletti, C., Maritan, A.
Folding Pathways of Prion and Doppel
*Biophys J.* **2002** Dec;83(6):3533-41.

Visintin, M., **Settanni, G.**, Graziosi, S., Maritan, A., Marks, J.D., Cattaneo, A.
The intracellular antibody capture technology (IACT): towards an optimal consensus sequence for intracellular antibodies.
*J. Mol. Biol.* **2002** 317 (1): 73-83

**Settanni G**, Cattaneo A, Maritan A
The role of native-state topology in the stabilization of intracellular antibodies
*Biophys. J.* **2001** 81: 2935-2945

Dima[+] RI, **Settanni[+] G**, Micheletti C, Banavar JR, Maritan A
Extraction of interaction potentials between amino acids from native protein structures
*J Chem Phys* 112: (20) 9151-9166 May 22 **2000**
[+] These two authors equally contributed to the work

**Settanni G**, Treves A
Analytical model for the effects of learning on spike count distributions
*Neural Comput* 12: (8) 1773-1787 Aug **2000**

## Refereed Conference papers

Uk B., M. Taufer, T. Stricker, **G. Settanni**, A. Cavalli, A. Caflisch
Combining Task- and Data Parallelism to Speed up Protein Folding on a Desktop Grid Platform
*Proc. of the CCGRID 2003,* IEEE International Symposium on Cluster Computing and the Grid, May **2003**, Tokyo, Japan.

Uk B., M. Taufer, T. Stricker, **G. Settanni**, A. Cavalli
Implementation and Characterization of Protein Folding on a Desktop Computational Grid
*Proc. of IPDPS 2003*, IEEE/ACM International, Parallel and Distributed Processing Symposium, April **2003**, Nice, France.

## Book Chapters

Schäfer, T; Muhl, C; Barz, M; Schmid, F; **Settanni**, G; Thermodynamics and Kinetics of the Interactions Between Proteins and Hydrophilic Polymers
High Performance Computing in Science and Engineering'19 (**2021**) 65-76, Springer, Cham

Schafer, T; Muhl, C; Barz, M; Schmid, F; **Settanni**, G;
Interactions Between Blood Proteins and Nanoparticles Investigated Using Molecular Dynamics Simulations
High Performance Computing in Science and Engineering'18(**2019**) 63-74, Springer, Cham

Schäfer, T; Zhou, J; Schmid, F; **Settanni**, G;
Blood Proteins and Their Interactions with Nanoparticles Investigated Using Molecular Dynamics Simulations
High Performance Computing in Science and Engineering'17(**2018**) Springer, Cham

Köhler, S; Schmid, F; **Settanni**, G;
The Internal Dynamics and Early Adsorption Stages of Fibrinogen Investigated by Molecular Dynamics Simulations
High Performance Computing in Science and Engineering´ 16, **2016**, 61-78, Springer, Cham

**Settanni G**.
Simulations and experiments in protein folding
*Molecular modelling of proteins, 2nd Edition,* **2015**; Kukol A. Editor, Humana press.

Köhler, S; Schmid, F; **Settanni**, G;
The Flexibility of Fibrinogen and its Initial Adsorption Stages at the Graphite and Mica Surface NIC Symposium 2014-Proceedings: 12–13 February 2014| Jülich, Germany, 117, **2014**, Forschungszentrum Jülich

Rao F., **Settanni G**., Caflisch A.
Estimation of folding probabilities and phi values from molecular dynamics simulations of reversible Peptide folding.
*Methods Mol Biol.* **2007**; 350:225-49.

## Other Publications

### Patents

Rabbits T.H., **Settanni G.**, Maritan A., Cattaneo A., Visintin M.
Intracellualr Antibodies. **2003**. Patent number WO03014960.