# **CURRICULUM VITAE**

# JOOST DE GRAAF

MIDDELBURG: JUNE 2, 1985

# CURRENT WORK ADDRESS

Institute for Theoretical Physics	Building	:	Buys Ballot Building 7.75
Department of Physics	STREET	:	Princetonplein 5
Faculty of Science	CITY	:	3584 CC Utrecht
Utrecht University	COUNTRY	:	The Netherlands
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#### **RESEARCH POSITIONS**

presently	Assistant Professor (UD1) Theory and Simulation of Soft Matter, Hydrodynamics, and Biophysics Utrecht University, Institute for Theoretical Physics, The Netherlands
2018 - 21	<b>Tenure-Track Assistant Professor (UD2)</b> <i>Theory and Simulation of Soft Matter, Hydrodynamics, and Biophysics</i> Utrecht University, Institute for Theoretical Physics, The Netherlands
2015 - 17	Marie Skłodowska-Curie Fellow University of Edinburgh, Institute for Condensed Matter and Complex Systems, Scotland
2015 - 15	<b>Group Leader</b> Active Matter and Anisotropic Colloids University of Stuttgart, Institute for Computational Physics, Germany
2012 - 14	Rubicon Postdoctoral research associate mentored by Prof. C. Holm University of Stuttgart, Institute for Computational Physics, Germany
2008 - 12	PhD Student supervised by Prof. M. Dijkstra Utrecht University, Debye Institute for Nanomaterials Science, Netherlands

# SCHOLARSHIPS AND GRANTS

- 2024 29 ITN *CoCoGel* (16 PI consortium; co-applicant), 4 year funding for a PhD student, Utrecht University, Netherlands
- 2021 24 NWO Klein (presently M1) Grant (single PI), 4 year funding for a PhD student, Utrecht University, Netherlands
- 2019 24 NWO Start-Up Grant (single PI), 5 year funding for a PhD student and 2-year postdoc, Utrecht University, Netherlands
- 2017 20 DFG SPP1726 Grant (author/unnamed co-PI<sup>1</sup>), 3 year funding for a PhD student, University of Stuttgart, Germany
- 2015 17 Marie Skłodowska-Curie Personal Fellowship (personal), 2 years, University of Edinburgh, Scotland
- 2014 17 DFG SPP1726 Grant (author/named co-PI), 3 year funding for a PhD student, University of Stuttgart, Germany
- 2013 15 NWO Rubicon Postdoctoral Scholarship (personal), 2 years, University of Stuttgart, Germany

<sup>&</sup>lt;sup>1</sup>Wrote most of the grant proposal. Working in the UK at the time barred me from being a named co-applicant.

#### DEGREES AND QUALIFICATIONS

 SKO (Senior Teaching Qualification), Utrecht University, Netherlands
 BKO (Basic Teaching Qualification), Utrecht University, Netherlands
 Ph.D in Physics cum laude, Utrecht University, Netherlands
 Supervisor: Prof. M. Dijkstra & René van Roij Thesis: Anisotropic Nanocolloids: Self-Assembly, Interfacial Adsorption, and Electrostatic Screening
 M.Sc. in Physics cum laude, Utrecht University, Netherlands
 B.Sc. in Physics and Mathematics cum laude, Utrecht University, Netherlands

#### ACADEMIC IMPACT

Number of citations <sup>2</sup>	:	2885	:	2179
h-index	:	28	:	23

#### ACADEMIC INTERESTS

My background is in the Statistical Mechanics of Soft-Matter systems. I am an expert in simulations involving hydrodynamic transport. My current research focuses on hydrodynamic interactions in passive and active systems, phoresis and osmosis mediated through (ionic) solute fields, viscoelastic fluids, complex out-of-equilibrium phenomena in dense fluids. Topics of interest include: colloidal gels, colloidal glasses, bacterial colonies, self-propelled particles, tesselation and geometry, jamming, tissue development, pattern formation due to chemical reactions.

#### ACADEMIC SPECIALITIES

Lattice-Boltzmann, Stokesian Dynamics, Monte Carlo, Molecular Dynamics, Crystal-Structure Prediction, Ewald Sums, Finite Element Methods, Analytic Electrokinetics, Classical Density Functional Theory, Free-Energy Calculations, Interfacial Adsorption, C++ and C Programming, CUDA Programming, WaLBerla, PyStencils, LBmPy, COMSOL, Mathematica, Linux, and Latex.

# OTHER PROFESSIONAL ACTIVITIES

- I am a reviewer for Science Advances, Reviews of Modern Physics, Physical Review Letters, Journal of Rheology, Soft Matter, Physical Review E, The Journal of Chemical Physics, The European Physics Journal E, *etc.* I am also reviewer for ERC (Starting Grants), NWO (Projectruimte), DFG individual grants, and PhD theses.
- Coordinator of the Master's program Theoretical Physics (2018 onward; presently focusing only on the double-degree students), Coordinator of the double degree Bachelor's thesis projects (2019 onward), Data management officer of the Institute for Theoretical Physics (2019 onward), PhD Counselor for the Physics Department (2022 onward), Co-Organizer of the Departmental Open Day (2022 onward), and sub-editor for the newsletter FYLAKRA (2018-2022).
- Outreach via *Pint of Science* (2020); via the Utrecht University initiative the Rector's League (2021 & 2019); via a talk at the Utrecht Physics Society (2019); at the Weekend van de Wetenschap (2018 & 2019), funded by the Utrecht University *Public Engagement Seed Fund* program; and at the National Museum for Edinburgh Science Festival (2016), *Demonstration with Mechanical Swimmer Models*.
- Lecturer of Statistical Physics at the National Physics Olympiad prep. classes (2020, 2021, & 2022). Prepared problems for the 2023 "Project Interuniversitaire Olympiade Natuurkunde."

<sup>&</sup>lt;sup>2</sup>Scopus & Google Scholar, respectively, 21.12.2023. It is useful to note that Scopus has a higher variance in the citation numbers reported, *i.e.*, the previous sampling point in december 2022 indicated 2500 citations.

### LANGUAGES

Dutch (native, C2) French (basic, A2) English (fluent, C2) Spanish (learning) German (proficient, B1)

# HOBBIES

Baking and cooking, cinema with an emphasis on 80s films, and cycling.

#### ORGANIZING WORKSHOPS/SCHOOLS, INVITED TALKS, AND INVITED LECTURES

- 16. Computational Advances in Active Matter, Leiden, Dec. 11 Dec. 15, 2023 Organized together with Prof. Drs. T.N. Shendruk, S. Henkes, and J. Stenhammar
- 15. European Colloid & Interface Society Conference, Chania, Sept. 04 Sept. 09, 2022 Talk: Understanding enhanced rotational dynamics of active probes in rod suspensions
- 14. Computational methods and tools for complex suspensions, Bilbao, May 23 May 27, 2022 Talk: Understanding enhanced rotational dynamics of active probes in rod suspensions
- 13. Interdisciplinary Challenges in Nonequilibrium Physics, online, Apr. 12 Apr. 16, 2021 Talk: Probing Glassy Colloidal Systems with Active Particles
- 12. ITN Numerical Methods of Active Matter, Lisbon, Portugal, Jan. 18 Feb. 04, 2021 Lecture: Advanced MD methods + wrote book chapter
- 11. 27th Dutch Soft Matter Meeting, Utrecht, Netherlands, November 05, 2019 Organized together with L. Filion
- 10. Statistical Mechanics of Active Matter School, L'Aquila, Italy, June 12-14, 2019 Lecture: Recognizing the Role of the Boundary
- 9. CECAM/ESBA 2019 workshop, Laursanne, Switzerland, July 25-27, 2019 Organized together with A. Morozov + a talk on gelation
- 8. Simulating Soft and Active Matter with ESPResSo, ESPResSo++, and VOTCA, Stuttgart, Germany, Oct. 08-12, 2018 Lecture on active matter
- 7. 24th Dutch Soft Matter Meeting, Leiden, Netherlands, June 8, 2018 Talk: The Impact of Hydrodynamics on Colloidal Gel Collapse
- 6. Simulating Soft and Active Matter with ESPResSo, ESPResSo++, and VOTCA, Stuttgart, Germany, Oct. 09-13, 2017 Lecture on active matter
- 5. Microswimmers International Conference, Bonn, Germany, Oct. 04-07, 2016 Talk: Lattice-Boltzmann Methods for Autophoretic Swimmers
- 4. Simulating Soft and Active Matter with ESPResSo, ESPResSo++, and VOTCA, Stuttgart, Germany, Oct. 05-09, 2015 Co-organizer and provided a lecture on active matter simualtions
- 3. The Future of Multi-Scale Soft Matter Modelling, Leiden, Netherlands, Aug. 31 Sept. 04, 2015 Talk: Towards Simulating Collective Motion of Chemically Self-Propelled Colloids
- 2. Micro- and NanoMachines, Hannover, Germany, July 02-05, 2014 Talk: Catalytically driven anisotropic self-propelled colloids
- 1. 11th Dutch Soft Matter Meeting, Eindhoven, Netherlands, Nov. 07, 2011 Talk: Hierarchical Self-Assembly of Suspended Branched Colloidal Nanocrystals into Super-Lattice Structures

# TEACHING

- Soft and Active Matter Theory (1 quadmester M.Sc.-level course), taught by R. van Roij and J. de Graaf, 2023, Utrecht University, Netherlands
- Advanced Statistical Mechanics (1 semester B.Sc.-level course), taught by J. de Graaf, 2023, Utrecht University, Netherlands

- Soft Matter Theory (1 semester M.S.-level course), taught by R. van Roij and J. de Graaf, 2022, Utrecht University, Netherlands
- Advanced Statistical Mechanics (1 semester B.Sc.-level course), taught by <u>J. de Graaf</u>, 2022, Utrecht University, Netherlands
- *Student Seminar Theoretical Physics* (1 semester M.Sc.-level course), coordinated by <u>J. de Graaf</u> and T. Hinderer, 2021, Utrecht University, Netherlands
- Advanced Statistical Mechanics (1 semester B.Sc.-level course), taught by <u>J. de Graaf</u>, 2021, Utrecht University, Netherlands
- *Student Seminar Theoretical Physics* (1 semester M.Sc.-level course), coordinated by <u>J. de Graaf</u>, 2020, Utrecht University, Netherlands
- Advanced Statistical Mechanics (1 semester B.Sc.-level course), taught by <u>J. de Graaf</u>, 2020, Utrecht University, Netherlands
- *Student Seminar Theoretical Physics* (1 semester M.Sc.-level course), coordinated by <u>J. de Graaf</u>, 2019, Utrecht University, Netherlands
- Advanced Statistical Mechanics (1 semester B.Sc.-level course), taught by L. Filion and <u>J. de Graaf</u>, 2019, Utrecht University, Netherlands
- *Advanced Topics in Theoretical Physics* (a 5 week module of a M.Sc.-level course on CFD), taught by <u>J. de Graaf</u>, 2019, Utrecht University, Netherlands
- Advanced Simulation Methods (1 semester course, comprised of four three-week modules), taught by C. Holm, <u>J. de Graaf</u>, J. Smiatek, and M. Fyta, 2015, University of Stuttgart, Germany
- *Hauptseminar Active Matter* (1 semester course; weekly lectures), organized by C. Holm, C. Bechinger, <u>J. de Graaf</u>, and J. Gomez-Solano, 2015, University of Stuttgart, Germany

# ONGOING (CO-)SUPERVISION OF STUDENTS

Students for whom I am the principle supervisor are in bold face.

2023 - **	I. Degroote, B.Sc. Student at Utrecht University, Netherlands Co-supervised by J.E. Frank (Mathematical Science, Utrecht University) Project: Sedimentation of Colloidal Chiral Objects
2023 - **	P. Michels, M.Sc. Student at Utrecht University, Netherlands Co-supervised by D. Panja (Computing Science, Utrecht University) Project: <i>FFTW-based CFD for Soft Matter Systems</i>
2023 - **	T. Womack, M.Sc. Student at Utrecht University, Netherlands Co-supervised by T.N. Shendruk (University of Edinburgh) Project: <i>Smectodynamics of Dividing Cells</i>
2023 - **	M. van Schaik, M.Sc. Student at Utrecht University, Netherlands Co-supervised by K.W. Torre (Institute for Theoretical Physics, Utrecht University) Project: <i>Coarse-grained modelling of gravitational gel collapse</i>
2023 - 24	<b>M. Toos</b> , PhD Guest Researcher Project: <i>The Dynamics of Oscillating Tissues</i>
2023 - **	B. Verhoef, PhD Candidate at Utrecht University, Netherlands Co-supervised by R. Hermsen (Theoretical Biology, Utrecht University) Project: <i>Resistance in Spatially Structured Bacterial Colonies</i>
2023 - **	<b>H. Nemati</b> , PhD Candidate at Utrecht University, Netherlands Project: <i>Living Tissues and their Dynamics</i>
2021 - **	<b>K.W. Torre</b> , PhD Candidate at Utrecht University, Netherlands Project: <i>The Role of Friction in Colloidal Gel Stability</i>
2019 - **	<b>M. Bos</b> , PhD Candidate at Utrecht University, Netherlands Project: <i>Turning through disorder:</i> <i>Models of bundled mucus strands and microswimmers</i>

#### COMPLETED (CO-)SUPERVISION OF STUDENTS AND RESEARCHERS

Students for whom I was the principle supervisor are in bold face.

- 2023 23 **E. Sijl**, B.Sc. Student at Utrecht University, Netherlands Project: *Models of Ca*<sup>2+</sup> *Spiking in Cilia: Toward Modeling Left-Right Differentiation*
- 2022 23 **B. Verhoef**, M.Sc. Student at Utrecht University, Netherlands Project: *Effect of Confinement on Bacterial Colony Growth*
- 2022 23 V. van Zwieten, M.Sc. Student at Utrecht University, Netherlands Co-supervised by D. Panja (Computing Science, Utrecht University) Project: *Bringing GPU Parallelization and Complex Boundaries to a Computational Fluid Dynamics Solver*
- 2022 22 **K. Sjöstedt**, Complex-Systems Project Student at Utrecht University, Netherlands Co-supervised by D. Panja (Computing Science, Utrecht University) Project: *Morphology and Characterisation of Bacterial Colonies Confined to Petri Dishes*
- 2021 23 **J. Roberts**, PhD Project at Utrecht University, Netherlands Co-supervised by F. Jafarpour (Institute for Theoretical Physics, Utrecht University) Project: *Understanding Bacterial Colony Growth using Machine Learning* Terminated PhD prematurely
- 2021 23 F. Gaeremynck, M.Sc. Student at Utrecht University, Netherlands Co-supervised by D. Panja (Computing Science, Utrecht University) Project: Improved methods on GPU-based versatile and efficient hydrodynamics code for scientific applications
- 2021 22 H. Leeuwis, M.Sc. Student at Utrecht University, Netherlands
   Co-supervised by J. Roberts (Institute for Theoretical Physics, Utrecht University)
   Co-supervised by D. Panja (Computing Science, Utrecht University)
   Project: Identifying PDEs in Interacting Particle Systems using Data-Driven Techniques
- 2021 22 M. van Leeuwen, B.Sc. Student at Utrecht University, Netherlands Co-supervised by J.E. Frank (Mathematical Science, Utrecht University) Co-supervised by K.W. Torre (Institute for Theoretical Physics, Utrecht University) Project: *Toward Understanding the Impact of the Meniscus on the Dynamics* of a Colloidal Gel using Continuum Models
- 2021 22 M. Brouwer, B.Sc. Student at Utrecht University, Netherlands Co-supervised by C. Oosterlee (Mathematical Science, Utrecht University) Co-supervised by B. Négyesi (Mathematical Science, Utrecht University) Project: Applying Physics-informed Neural Networks to Chaotic Nonlinear Systems of Ordinary Differential Equations
- 2021 22 T. Schouten, B.Sc. Student at Utrecht University, Netherlands Co-supervised by P. Salanevich (Mathematical Science, Utrecht University) Co-supervised by D. Brunner (Skope, Zurich, Switzerland) Project: Under Embargo due to Non-Disclosure Agreement with Skope
- 2020 21 J. Roberts, double-degree M.Sc. Student at Utrecht University, Netherlands Co-supervised by D. Valesin (Mathematical Science, University of Groningen) Corrected by W. Ruszel (Mathematical Science, Utrecht University) Project: Asymptotic Shape of a One-Dimensional Growth Process in a Dynamic Environment
- 2020- 21 B. Stam, M.Sc. Student at Utrecht University, Netherlands Co-supervised by D. Panja (Computing Science, Utrecht University) Project: A GPU-based versatile and efficient hydrodynamics code for scientific applications

- 2019 22 M. Palusa, PhD Student at the University of Edinburgh, Scotland Promotor: A. Morozov (University of Edinburgh) Project: *Dynamics of Chiral Particles in Viscous Fluids*
- 2019 20 R. Meijer, B.Sc. Student at Utrecht University, Netherlands
   Co-supervised by: M. Ries (Biomedical Imaging, University Medical Center Utrecht)
   Project: A numerical study on the sub- and ultraharmonic response of
   an oscillating microbubble in a rigid tube
- 2019 20 **R. Hardeman**, B.Sc. Student at Utrecht University, Netherlands Project: *Modeling viscosity-dependent reversal of fluid transport driven by magnetic cilia*
- 2019 20 **T. ter Rele**, B.Sc. Student at Utrecht University, Netherlands Co-supervised by M. Bos (Institute for Theoretical Physics, Utrecht University) Project: *Modelling the Dynamics of Epithelial Tissue*
- 2019 20 **C. Wiggers**, B.Sc. Student at Utrecht University, Netherlands Co-supervised by M. Bos (Institute for Theoretical Physics, Utrecht University) Project: *Growth Process of Disk- and Rod- Shaped Bacterial Colonies in 2D*
- 2019 20 **B. van den Bosch**, B.Sc. Student at Utrecht University, Netherlands Project: *Minimal model of a nodal cilium*
- 2019 20 **C. Perugachi Israëls**, B.Sc. Student at Utrecht University, Netherlands Project: *Cilia-induced Flow in the Embryonic Node of Mice and Asymmetric Gene Expression*
- 2019 20 **C. Abaurrea Velasco**, Postdoc at Utrecht University, Netherlands Project: *Self-propelled Particles in Viscoelastic Media*
- 2018 19 **M. Inês Cravo**, M.Sc. Student at Utrecht University, Netherlands Project: *Cellular Oscillations in Models of Biological Tissues*
- 2018 18 C. Stewart, M.Sc. Student at the University of Stuttgart, Germany Supervised by M. Kuron (Institute for Computational Physics, University of Stuttgart) Co-Supervised by C. Holm (Institute for Computational Physics, University of Stuttgart) Project: *Simulating Viscoelastic Media using Lattice-Boltzmann*
- 2018 18 P. Stärk, B.Sc. Student at the University of Stuttgart, Germany Supervised by M. Kuron (Institute for Computational Physics, University of Stuttgart) Co-Supervised by C. Holm (Institute for Computational Physics, University of Stuttgart) Project: *Toward Swimming in Porous Networks:* Interactions Between Microswimmers and Obstacles
- 2017 22 T. Welling, PhD Student at Utrecht University, Netherlands Promotor: A. van Blaaderen (Debye Institute, Utrecht University) Co-supervised by M. van Huis (Debye Institute, Utrecht University) Project: Rattle-type particles: Tuning colloidal interactions and electrokinetics for switchable colloidal crystals
- 2017 17 **M. Haughey**, Senior Honours Student at the University of Edinburgh, Scotland Project: *Simulating Hydrodynamic Flow during the Collapse of Colloidal Gels*
- 2016 21 **M. Kuron**, PhD Student (Magna cum Laude) at the University of Stuttgart, Germany Promotor: C. Holm (Institute for Computational Physics, University of Stuttgart) Project: Lattice-Boltzmann Methods for Microswimmers in Complex Environments
- 2016 17 **H. Menke**, Student Assistant at the University of Stuttgart, Germany Project: *Discrete Self-Electrophoretic Self-Propelled Nanoparticles*
- 2016 16 R. Pruciak, Senior Honours Student shared with University of Edinburgh, Scotland Co-supervised by A. Brown (Deptartment of Physics, University of Edinburgh) Project: *The Fluid Dynamics of Sedimenting Helices (Experimental)*

- 2016 16 B. Droste, M.Sc. Student at the University of Utrecht, Netherlands Supervised by M. Dijkstra (Debye Institute, Utrecht University) Project: Sedimentation of One and Two Helices including Hydrodynamic Interactions
- 2015 16 **P. Kreissl**, M.Sc. Student at the University of Stuttgart, Germany Project: *Autophoretic Mechanisms: Efficiency, Interactions, and Geometry*
- 2015 15 S. Ehrhardt, M.Sc. Student at the University of Stuttgart, Germany Co-supervisor: G. Rempfer (Institute for Computational Physics, University of Stuttgart) Project: Simulation of Electroosmotic Flow through Nanocapillaries using Finite-Element Methods
- 2015 15 M. Kuron, M.Sc. Student at the University of Stuttgart, Germany Co-supervisor: G. Rempfer (Institute for Computational Physics, University of Stuttgart) Project: Efficient Lattice-Boltzmann Algorithms for Colloids Undergoing Electrophoresis
- 2015 15 **S. Ilse**, B.Sc. Student at the University of Stuttgart, Germany Project: *Motility Induced Phase Separation of Active Triangles with Surface Roughness*
- 2015 15 **F. Schultz**, B.Sc. Student at the University of Stuttgart, Germany Project: *The Liquid-Crystal Phase Coexistence in Systems Doped with Active Particles*
- 2015 15 **M. Fabritius**, Project Student at the University of Stuttgart, Germany Project: *Self-Propelled Particles near Flat and Curved Boundaries*
- 2014 16 G. Rempfer, PhD Student at the University of Stuttgart, Germany Promotor: C. Holm (Institute for Computational Physics, University of Stuttgart) Project: *Simulating Nanopores using Lattice-Based Electrokinetic Algorithms*
- 2014 14 L. Fischer, B.Sc. Student at the University of Stuttgart, Germany Project: Brownian Translation and Rotational Diffusion of anisotropic Colloids in cubic crystals: A Lattice-Boltzmann study of the Hydrodynamic Coupling with application to Rotator Phases
- 2014 14 **T. Peter**, B.Sc. Student at the University of Stuttgart, Germany Project: Brownian Translational and Rotational Diffusion of a Spherical Colloid in Quasi-Two-Dimensional Confinement: A Lattice-Boltzmann Study of the Properties of the Raspberry Model
- 2011 11 E. Hildebrandt, M.Sc. Student at Utrecht University, Netherlands Co-supervised by M. Dijkstra (Debye Institute, Utrecht University) Co-supervised by R. Bisseling (Mathematical Science, Utrecht University) Project: *Towards Simulation Studies of Crystal Structures for Superellipsoids by Floppy Box Monte Carlo Method*

Summarizing, I have presently (co-)supervised 1 Postdoc; 10 PhD Candidates, of which 4 are still working toward their thesis, 1 is a guest researcher, and 1 terminated their program prematurely; 16 M.Sc.-level students, of which 3 are working on their project; 20 B.Sc.-level students, of which 1 is working on their project; and one student assistant.

# PEER-REVIEWED PAPERS

Please note that all paper titles below are hyperlinked to the relevant journal page.

- 58. M. Bos, A. Ermund, G. Hansson, and <u>J. de Graaf</u>, *Goblet cell interactions reorient bundled mucus strands for efficient airway clearance*, PNAS Nexus **2**, pgad388 (2023)
- 57. K. Torre and <u>J. de Graaf</u>, *Hydrodynamic Lubrication in Colloidal Gels*, Soft Matter **19**, 7388 (2023)
- 56. <u>J. de Graaf</u>, K. Torre, W. Poon, and M. Hermes, *Hydrodynamic stability criterion for colloidal gelation under gravity*, Phys. Rev. E **107**, 034608 (2023)
- 55. K. Torre and <u>J. de Graaf</u>, *Structuring Colloidal Gels via Micro-Bubble Oscillations*, Soft Matter **19**, 2771 (2023)

- 54. T. Welling, A. Grau-Carbonell, K. Watanabe, D. Nagao, <u>J. de Graaf</u>, M. van Huis, and A. van Blaaderen, *Frequency-controlled electrophoretic mobility of a particle within a porous, hollow shell*, J. Colloid Interface Sci. **627**, 761 (2022)
- 53. N. Narinder, M. Bos, C. Abaurrea-Velasco, <u>J. de Graaf</u>, and C. Bechinger, *Understanding enhanced rotational dynamics of active probes in rod suspensions*, Soft Matter **18**, 6246 (2022)
- 52. S. Ketzetzi, M. Rinaldin, P. Dröge, <u>J. de Graaf</u>, and D. Kraft, *Activity-induced microswimmer interactions and cooperation in one-dimensional environments*, Nat. Commun. **13**, 1772 (2022)
- A. Demirörs, S. Aykut, S. Ganzeboom, Y. Meier, R. Hardeman, <u>J. de Graaf</u>, A. Mathijssen, E. Poloni, J. Carpenter, C. Ünlü, and D. Zenhäusern, *Amphibious Transport of Fluids and Solids by Soft Magnetic Carpets*, Sci. Adv. **8** 2102510 (2021)
- 50. T. Welling, K. Watanabe, A. Grau-Carbonell, <u>J. de Graaf</u>, D. Nagao, A. Imhof, M. van Huis, and A. van Blaaderen, *Tunability of interactions between the core and shell in rattle-type particles studied with liquid-cell electron microscopy*, ACS Nano **15**, 11137 (2021)
- 49. T. Huang, B. Ibarlucea, A. Caspari, A. Synytska, G. Cuniberti, <u>J. de Graaf</u>, and L. Baraban, *Impact of surface charge on the motion of light-activated Janus micromotors*, Euro. Phys. J. E **44**, 39 (2021)
- M. Kuron, C. Stewart, <u>J. de Graaf</u>, C. Holm, *An extensible lattice Boltzmann method for vis-coelastic flows: complex and moving boundaries in Oldroyd-B fluids*, Euro. Phys. J. E 44, 1 (2021)
- A. Demirörs, A. Stauffer, C. Lauener, J. Cossu, S. Ramakrishna, <u>J. de Graaf</u>, C. Alcantara, S. Pané, N. Spencer, A. Studart, *Magnetic propulsion of colloidal microrollers controlled by electrically modulated friction*, Soft Matter **17**, 1037 (2021)
- 46. R. Verweij, S. Ketzetzi, <u>J. de Graaf</u>, and D. Kraft, *Height distribution and orientation of colloidal dumbbells near a wall*, Phys. Rev. E **102**, 062608 (2020)
- 45. C. Abaurrea-Velasco, C. Lozano, C. Bechinger, and <u>J. de Graaf</u>, *Autonomously Probing Viscoelasticity in Disordered Suspensions*, Phys. Rev. Lett. **125**, 258002 (2020)
- 44. S. Ketzetzi, <u>J. de Graaf</u>, and D. Kraft, *Diffusion-based height analysis reveals robust micro-swimmer-wall separation*, Phys. Rev. Lett. **125**, 238001 (2020)
- 43. S. Ketzetzi, <u>J. de Graaf</u>, R. Doherty, and D. Kraft, *Slip length dependent propulsion speed of catalytic colloidal swimmers near walls*, Phys. Rev. Lett. **124**, 048002 (2020)
- 42. Z. Zhang, <u>J. de Graaf</u>, and S. Faez, *Regulating the aggregation of colloidal particles in an electro-osmotic micropump*, Soft Matter **16**, 10707 (2020)
- 41. <u>J. de Graaf</u> and S. Samin, *Self-thermoelectrophoresis at low salinity*, Soft Matter **15**, 7219 (2019)
- 40. M. Kuron, P. Stärk, C. Holm, and <u>J. de Graaf</u>, *Hydrodynamic Mobility Reversal of Squirmers near Flat and Curved Surfaces*, Soft Matter **15**, 5908 (2019)
- 39. M. Kuron, P. Stärk, <u>J. de Graaf</u>, and C. Holm, *A Lattice Boltzmann Model for Squirmers*, J. Chem. Phys. **150**, 144110 (2019)
- 38. <u>J. de Graaf</u>, W.C.K. Poon, M.J. Haughey, and M. Hermes, *Hydrodynamics strongly affect the dynamics of colloidal gelation but not gel structure*, Soft Matter **15**, 10 (2019)
- F. Weik, R. Weeber, K. Szuttor, K. Breitsprecher, <u>J. de Graaf</u>, M. Kuron, J. Landsgesell, H. Menke, D. Sean, and C. Holm, *ESPResSo 4.0 – An Extensible Software Package for Simulating Soft Matter Systems*, Eur. Phys. J. S.T. **227**, 1789 (2019)
- 36. M. Palusa, <u>J. de Graaf</u>, A. Brown, and A. Morozov, *Sedimentation of a rigid helix in viscous media*, Phys. Rev. Fluids **3**, 124301 (2018)
- 35. A. Castelli, <u>J. de Graaf</u>, S. Marras, R. Brescia, L. Goldoni, L. Manna, and M. Arciniegas, *Understanding and Tailoring Ligand Interactions in the Self-Assembly of Branched Colloidal Nanocrystals into Planar Superlattices*, Nat. Commun. **9**, 1141 (2018)
- 34. R. Niu, P. Kreissl, A. Brown, G. Rempfer, D. Botin, C. Holm, T. Palberg, and <u>J. de Graaf</u>, *Microfluidic Pumping by Micromolar Salt Concentrations*, Soft Matter **13**, 1505 (2017)
- 33. A. Brown, W. Poon, C. Holm, and <u>J. de Graaf</u>, *Ionic Screening and Dissociation are Crucial for* Understanding Chemical Self-Propulsion in Polar Solvents, Soft Matter **13**, 1200 (2017)
- G. Rempfer, S. Ehrhardt, C. Holm, and <u>J. de Graaf</u>, Nanoparticle Translocation through Conical Nanopores: A Finite Element Study of Electrokinetic Transport, Macromol. Theor. Simul. 26, 1600051 (2017)

- 31. J. de Graaf and J. Stenhammar, Lattice-Boltzmann Simulations of Microswimmer-Tracer Interactions, Phys. Rev. E 95, 023302 (2017)
- M. Kuron, G. Rempfer, F. Schornbaum, M. Bauer, C. Godenschwager, C. Holm, and <u>J. de Graaf</u>, Moving Charged Particles in Lattice Boltzmann-Based Electrokinetics, J. Chem. Phys. **145**, 214102 (2016)
- 29. <u>J. de Graaf</u> and J. Stenhammar, *Stirring by Periodic Arrays of Microswimmers*, J. Fluid Mech. **811**, 487 (2016)
- 28. S. Ilse, C. Holm, and <u>J. de Graaf</u>, *Surface Roughness Stabilizes the Clustering of Self-Propelled Triangles*, J. Chem. Phys. **145**, 134904 (2016)
- 27. G. Rempfer, S. Ehrhardt, N. Laohakunakorn, G. Davies, U. Keyser, C. Holm, and <u>J. de Graaf</u>, *Selective Trapping of DNA Using Glass Microcapillaries*, Langmuir **32**, 8525 (2016)
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- 18. <u>J. de Graaf</u>, G. Rempfer, and C. Holm, *Diffusiophoretic Self-Propulsion for Partially Catalytic Spherical Colloids*, IEEE Trans. Nanobiosci. **14**, 272 (2015)
- 17. A. Gantapara, <u>J. de Graaf</u>, R. van Roij, and M. Dijkstra, *Phase Behavior of a Family of Truncated Hard Cubes*, J. Chem. Phys. **142**, 054904 (2015)
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- 15. M. Arciniegas, M. Kim, <u>J. de Graaf</u>, R. Brescia, S. Marras, K. Miszta, M. Dijkstra, R. van Roij, and L. Manna, *Self-Assembly of Octapod-Shaped Colloidal Nanocrystals into a Hexagonal Ballerina Network Embedded in a Thin Polymer Film*, Nano Lett. **14**, 1056 (2014)
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- 12. <u>J. de Graaf</u>, L. Filion, M. Marechal, M. Dijkstra, and R. van Roij, *Crystal-structure prediction via the Floppy-Box Monte Carlo algorithm: Method and application to hard (non)convex particles*, J. Chem. Phys. **137**, 214101 (2012)
- W. Evers, B. Goris, S. Bals, M. Casavola, <u>J. de Graaf</u>, R. van Roij, M. Dijkstra, and D. Vanmaekelbergh, *Low-Dimensional Semiconductor Superlattices Formed by Geometric Control over Nanocrystal Attachment*, Nano Lett. **13**, 2317 (2012)
- 10. <u>J. de Graaf</u>, N. Boon, M. Dijkstra, and R. van Roij, *Electrostatic Interactions between Janus Particles*, J. Chem. Phys. **137**, 104910 (2012)
- W. Qi, J. de Graaf, F. Qiao, S. Marras, L. Manna, and M. Dijkstra, Ordered Two-Dimensional Superstructures of Colloidal Octapod-Shaped Nanocrystals on Flat Substrates, Nano Lett. 12, 5299 (2012)

- 8. R. Ni, A. Gantapara, <u>J. de Graaf</u>, R. van Roij, and M. Dijkstra, *Phase Diagram of Colloidal Hard Superballs: from Cubes via Spheres to Octahedra*, Soft Matter **8**, 8826 (2012)
- 7. J. de Graaf, R. van Roij, and M. Dijkstra, *Dense Regular Packings of Irregular Nonconvex Particles*, Phys. Rev. Lett. **107**, 155501 (2011)
- K. Miszta, J. de Graaf, G. Bertoni, D. Dorfs, R. Brescia, S. Marras, L. Ceseracciu, R. Cingolani, R. van Roij, M. Dijkstra, and L. Manna, *Hierarchical Self-Assembly of Suspended Branched Colloidal Nanocrystals into Superlattice Structures*, Nat. Mater. **10**, 872 (2011)
- J. de Graaf, M. Dijkstra, and R. van Roij, Adsorption Trajectories and Free-Energy Separatrices for Colloidal Particles in Contact with a Liquid-Liquid Interface, J. Chem. Phys. 132, 164902 (2010)
- J. de Graaf, M. Dijkstra, and R. van Roij, *Triangular Tessellation Scheme for the Adsorption Free* Energy at the Liquid-Liquid Interface: Towards Nonconvex Patterned Colloids, Phys. Rev. E 80, 051405 (2009)
- 3. M. Bier, <u>J. de Graaf</u>, J. Zwanikken, and R. van Roij, *Curvature Dependence of the Electrolytic Liquid-Liquid Interfacial Tension*, J. Chem. Phys. **130**, 024703 (2009)
- J. de Graaf, J. Zwanikken, M. Bier, A. Baarsma, Y. Oloumi, M. Spelt and R. van Roij, Spontaneous Charging and Crystallization of Water Droplets in Oil, J. Chem. Phys. 129, 194701 (2008)
- 1. J. Zwanikken, <u>J. de Graaf</u>, M. Bier, and R. van Roij, *Stability of Additive-Free Water-in-Oil Emulsions*, J. Phys.: Condens. Matter **20**, 494238 (2008)

Scientific publication is unfortunately prone to errors. The responsible course of action is to report these and provide transparency, such that these do not affect other researchers. Here, I list those issues that I am aware of for the papers listed above.

In [W.H. Evers *et al.*, Nano Lett. **13**, 2317 (2012)] the proposed argument for the orientation of the nanocrystals is overly simplified, this model was subsequently improved upon in [G. Soligno, M. Dijkstra, and R. van Roij, Phys. Rev. Lett. **116**, 258001 (2016)].

Both papers on the raspberry-particle method for fluid coupling [J. de Graaf *et al.*, J. Chem. Phys. **143**, 084108 (2015) and L. Fischer *et al.*, J. Chem. Phys. **143**, 084107 (2015)] contain minor oversights that are corrected and identified in the latest *arXiv* versions of the manuscripts.

In [M. Kuron *et al.*, J. Chem. Phys. **150**, 144110 (2019)] we report lattice artefacts for a moving squimer. I suspect that the origin of these is a bug/inconsistency in the way boundary conditions are handled in the lattice-Boltzmann (LB) algorithm of **WalBerLa**, rather than something intrinsically wrong with implementing squimers in LB. This is because both for the electrokinetic version [M. Kuron *et al.*, J. Chem. Phys. **145**, 214102 (2016)] and the viscoelastic version of the LB method [M. Kuron *et al.*, Euro. Phys. J. E **44**, 1 (2021)], we were unable to get self-propelled particles or squimers to work properly. In fact, for the latter, there was a clear artefact, which depended sensitively on the direction in which the squirmer traversed the simulation box. In addition, snow-man-like swimmers in a viscoelastic LB medium came to a halt, rather than that they continued to move with a constant velocity. My current understanding is that there is a small bug in the working of the moving boundary conditions in **WalBerLa**, which is obscured by putting an external force on the object. Whenever the forces on the fluid are self-generated, as is the case with squirmers, this effect is much more noticeable. Squirmer particles in LB likely do not require the diameters that we report in [M. Kuron *et al.*, J. Chem. Phys. **150**, 144110 (2019)].

Finally, for [C. Abaurrea-Velasco *et al.*, Phys. Rev. Lett. **125**, 258002 (2020)] there was an oversight in terms of the referencing, which has been corrected *via* an erratum. In addition, it is my current understanding that the model that we used does not have a glass transition in the sense of the experimental system by the Bechinger group. That is, we misidentified the jamming transition as a glass transition. Nonetheless, the major elements of the paper hold, as can be appreciated from the follow-up study [N. Narinder *et al.*, Soft Matter **18**, 6246 (2022)].

#### OTHER PAPERS

3. M. Kuron, P. Kreissl, and C. Holm<sup>\*</sup>, *Toward Understanding of Self-Electrophoretic Propulsion under Realistic Conditions : From Bulk Reactions to Confinement Effects*, Acc. Chem. Res. **51**,

2998 (2018)

- 2. <u>J. de Graaf</u> and L. Manna<sup>†</sup>, *A Roadmap for the Assembly of Polyhedral Particles*, Science **337**, 417 (2012)
- M. Dijkstra, <u>J. de Graaf</u>, D. Vanmaekelbergh, and R. van Roij, *Orde uit wanorde: Van plantensex via Einstein naar zelf-assemblage van nanodeeltjes*, Nederlands Tijdschrift voor Natuurkunde **78**(7), 258 (2012)]

\*For the Accounts in Chemical Research, I wrote most of the SPP1726 grant, I co-supervised the research, wrote the conspectus, and reviewed part of the writing before submission. Unfortunately, I was forced to pull my name off the article, due to the way in which the writing of this manuscript was managed. For example, upon submission of the paper, the research that A. Brown had initiated on ionic screening for microswimmers and with which I was involved for the numerical aspects [A. Brown *et al.*, Soft Matter **13**, 1200 (2017)], was significantly misrepresented: trends that are due to swimmer size were attributed to bulk ionic reactions. I have, however, had the involved PhD candidates fix this post peer-review, against the wishes of the management. Please do not blame the PhDs for the clear misrepresentation of involvement or way the research came about.

<sup>†</sup>The Science publication is an editorial perspective on the work by the group of S. Glotzer. The vast majority of the writing was carried out by L. Manna.

# **REGULAR TALKS & POSTERS**

Talks at local events, such as invited seminars, colloquia, etc. are not listed here.

- 35. XIXth International Congress on Rheology, Athens, July 29 Aug. 04, 2023 Talk: Understanding enhanced rotational dynamics of active probes in rod suspensions
- 34. SoftComp Annual Meeting, Ancona, May 23 May 25, 2023 Talk: Understanding enhanced rotational dynamics of active probes in rod suspensions
- 33. New Perspectives in Active Systems, Dresden, April 24 April 28, 2023 Poster: Understanding enhanced rotational dynamics of active probes in rod suspensions
- 32. 2022 IFPRI Annual General Meeting, Leuven, Belgium, June 15, 2022 Poster: *Oscillating Micro-Bubbles in Colloidal Gels*
- 31. Iontronics, Utrecht, Netherlands, Oct. 11, 2019 Poster: *Self-Thermoelectrophoresis at Low Salinity*
- 30. 5th International Soft Matter Conference, Edinburgh, Scotland, June 3-7, 2019 Poster: *Flow-Induced Dynamic Stability of Colloidal Gelation under Gravity*
- 29. 40th IFPRI Meeting, Edinburgh, Scotland, June 18-22, 2018 Poster: *The Stability of Colloidal Gels: meniscus effects, hydrodynamics and two-component systems*
- 28. Thermodynamics Conference, Edinburgh, Scotland, September 5-7, 2017 Talk: *Fluid Flow speeds up the Gravitational Collapse of Colloidal Gels*
- 27. 10th Liquid Matter Conference, Ljubljana, Slovenia, July 17-21, 2017 Talk: *Fluid Flow speeds up the Gravitational Collapse of Colloidal Gels*
- 26. 26th International Conference on Discrete Simulation of Fluid Dynamics, Erlangen, Germany, July 10-14, 2017 Talk: *Fluid Flow speeds up the Gravitational Collapse of Colloidal Gels*
- 25. 39th IFPRI Meeting, Philadelphia, United States of America, June 18-22, 2017 Poster: *Gravity and Hydrodynamics join forces to destroy Colloidal Gels*
- 24. Microswimmers, Self-Propelled Particles, and Active Matter , Lausanne, Switzerland, March 6-8, 2017 Talk: *Lattice-Boltzmann Simulations of Chemical Swimmers with Bulk-Ionic Dissociation*
- 23. 4th International Soft Matter Conference, Grenoble, France, Sept. 12-16, 2016 Poster: Bulk Ionic Dissociation is Crucial for Understanding Chemically-Propelled Swimmers Poster: The Interplay of Geometry and Hydrodynamics: Understanding the Motion of Self-Propelled Particles and Tracers

- 22. Micro- and Nanomachines, Hannover, Germany, June 29 July 1, 2016 Poster: The Interplay of Geometry and Hydrodynamics: Understanding the Motion of Self-Propelled Particles and Tracers
- 24rd International Conference on Discrete Simulation of Fluid Dynamics, Edinburgh, Scotland, July 13-17, 2015 Talk: Lattice-Boltzmann Simulations of Self-Propelled Rods: Snaking through a Micro Channel
- 20. Microswimmers: from bulk to interfaces, Bordeaux, France, Apr. 13-15, 2015 Talk: *Lattice-Boltzmann Simulations of Self-Propelled Rods: Snaking through a Micro Channel*
- 23rd International Conference on Discrete Simulation of Fluid Dynamics, Paris, France, July 28 - Aug. 01, 2014 Talk: *Catalytically driven anisotropic self-propelled colloids*
- 18. 9th Liquid Matter Conference, Lisbon, Portugal, July 21-25, 2014 Poster: *Catalytically Driven Anisotropic Self-Propelled Colloids: Janus Spheres and Conical Swimmers*
- 17. 3rd International Soft Matter Conference, Rome, Italy, Sept. 16-19, 2013 Poster: Crystal Structure Prediction Using The Floppy-Box Monte Carlo Algorithm
- 16. SFB TR6 CODEF III, Bonn, Germany, Mar. 20-23, 2012 Talk: *Crystal Structure Prediction and Self-Assembly of Nonconvex Branched Nanoparticles and Colloids*
- 15. 12th Dutch Soft Matter Meeting, Amsterdam, Netherlands, Apr. 27, 2012 Soundbite: *Poisson-Boltzmann Theory and Monte Carlo Simulations for Charged Janus Dipoles*
- 14. Physics@FOM, Veldhoven, Netherlands, Jan. 17-18, 2012 Talk: *Hierarchical Self-Assembly of Suspended Branched Colloidal Nanocrystals into Superlattice Structures*
- 8th Liquid Matter Conference, Vienna, Austria, Sept. 06-10, 2011
   Poster: Predicting Crystal Structures and Phase Behavior of Faceted Non-Convex Colloids and Nanoparticles
   Poster: Monte Carlo and Poisson Boltzmann Studies of Heterogeneously Charged Colloids in an Electrolyte
   Poster: The Dynamics of Adsorption for Anisotropic Colloids near Liquid-Liquid Interfaces
- 12. 10th Dutch Soft Matter Meeting, Utrecht, Netherlands, May 23, 2011 Soundbite: *The Assembly of Octapod Nanocrystals into Chains and 3D Superstructures*
- 11. SFB TR6 Young Researcher Workshop, Utrecht, Netherlands, Apr. 18-19, 2011 Talk: *Triangular-Tessellation based Numerical Techniques and their Applications: Interfacial Adsorption and Crystal-Structure Prediction of Anisotropic Colloids*
- 10. Physics@FOM, Veldhoven, Netherlands, Jan. 18-19, 2011 Talk: *Triangular-Tessellation based Numerical Techniques and their Applications: Interfacial Adsorption and Crystal-Structure Prediction of Anisotropic Colloids*
- 9. 9th Dutch Soft Matter Meeting, Leiden, Netherlands, Nov. 24, 2010 Soundbite: *Triangular Tessellation: Crystal Structures of Anisotropic Particles*
- 8. NanoSeminar, Utrecht, Netherlands, Oct. 15, 2010 Talk: *Triangular-Tessellation in Colloid Science: Interfacial Adsorption and Crystal-Structure Prediction of Anisotropic Colloids*
- 7. 2nd International Soft Matter Conference, Granada, Spain, Jul. 05-08, 2010 Poster: *Towards the Dynamics of Colloid Adsorption to Liquid-Liquid Interfaces*
- 6. 8th Dutch Soft Matter Meeting, Wagening, Netherlands, Apr. 14, 2010 Soundbite: *Towards Adsorption Dynamics of Colloids at the Liquid-Liquid Interface*
- 5. IOP Complex Fluid-Fluid Interfaces, London, England, Feb. 25, 2010 Talk: *Towards Adsorption Dynamics of Colloids at the Liquid-Liquid Interface: an Application of the Triangular Tessellation Scheme*

- 4. NWO CW (Xth Dutch Polymer Days), Veldhoven, Netherlands, Feb. 15-16, 2010 Poster: Interfacial Adsorption Dynamics of Colloids: Application of the Triangular Tessellation Technique
- 3. Physics@FOM, Veldhoven, Netherlands, Jan. 20-21, 2010 Poster: Interfacial Adsorption Dynamics of Colloids: Application of the Triangular Tessellation Technique
- 2. SFB TR6 Young Researcher Workshop, Mainz, Germany, Nov. 26-27, 2009 Talk: *The Adsorption Mechanism of Colloids near the Liquid-Liquid Interface: a Triangular Tessellation Scheme*
- 1. Physics@FOM, Veldhoven, Netherlands, Jan. 20-21, 2009 Poster: *Near Oil-Water Interfaces: Towards Understanding Emulsion Stability*

INTERNATIONAL SCHOOLS AND WORKSHOPS ATTENDED

- 2022 CECAM: New frontiers in liquid matter, Paris, France
- 2022 Physics of Life Summer School, Edinburgh, Scotland
- 2022 CECAM: Recent advances on the glass problem, online
- 2018 *Machine Learning and Reverse Engineering for Soft Materials (Lorentz Workshop)*, Leiden, Netherlands
- 2018 Topology in Complex Fluids (Lorentz Workshop), Leiden, Netherlands
- 2017 Bio-Informulation 2017, Edinburgh, Scotland
- 2017 Higgs/SUPA meeting on non-equilibrium collective dynamics, Perth, Scotland
- 2016 Physical Principles of Biological and Active Systems, Edinburgh, Scotland
- 2015 *The Future of Multi-Scale Soft Matter Modelling (Lorentz Workshop)*, Leiden, Netherlands
- 2014 Active Particles and Microswimmers (MPI), Kreuth, Germany
- 2013 GPU Programming using CUDA (HLRS), Stuttgart, Germany
- 2012 ESPResSo Summer School (ICP), Stuttgart, Germany
- 2010 MolSim 2010 (UvA), Amsterdam, Netherlands
- 2009 Computer Simulation Approaches to Study Self-Assembly: From Patchy Nano-Colloids to Virus Capsids (CECAM), Lausanne, Switzerland
- 2009 *Mainz Materials Simulations Days 2009 (MPI)*, Mainz, Germany

#### **TEACHING ASSISTANTSHIPS**

- Summer School on Active and Flowing Soft Matter (a 5-day PhD-level summer school), organized by A. Morozov and C. Hooley, 2017, CM-CDT Higgs school, University of St. Andrews, Scotland
- Hauptseminar Theorie und Simulation der weichen Materie (1 semester course; weekly lectures), taught by C. Holm, J. Smiatek, M. Krüger, and M. Bier, 2014, University of Stuttgart, Germany
- Hauptseminar Theorie und Simulation der weichen Materie (1 semester course; weekly lectures), taught by C. Holm, J. Smiatek, M. Krüger, and M. Bier, 2013, University of Stuttgart, Germany
- *Thermische Fysica I* (1 semester course; weekly lectures), taught by R. van Roij and M. Dijkstra, 2008/2009, 2009/2010, and 2010/2011, Utrecht University, Netherlands
- *Electromagnetisme* (1/2 semester course; weekly lectures), taught by A. Imhof and C. Klaassen, 2010, Utrecht University, Netherlands