

2023 Wet Systems Consultant Report

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University of Delaware

2018 IFPRI workshop wet systems roadmap

Need

1. Mechanisms of suspension rheology and stability

How can rheology / flow / jamming be tailored, changed, altered, controlled? e.g. adsorbates, stabilizers, surface chemistry, particle properties (size distribution, shapes, roughness)



- Connecting structure, composition, particle characteristics to rheology and function (**Slurry and Paste Rheology, SIFS projects**)

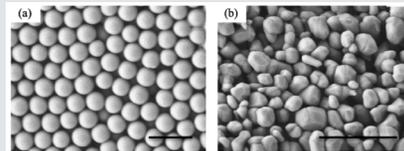
- Tailored rheology with interactions, particle roughness (see SIFS project update)

- **Missing: computational models**

2. Model formulations and model validation

"Is your adhesive hard sphere index-matched monodisperse suspension truly representative of my suspension?"

Effect of fines, polydispersity, roughness, shape, ...



Lee et al., 2020



- **SIFS project** with Jan Vermant (renewal) includes both bottom-up and top-down

- Collaboration with Lilian Hsiao (particle roughness)

- Vermant collaboration with Lucio Isa (particle friction, roughness)

3. Formulation and stability (especially involving changes)

Aging, *formulation changes, sensitivity, feed variability*

Predictable? "How close to edge" is a formulation?

"What can go wrong" / "what just went wrong"?

Informs accelerated testing? (*months / years to days / weeks*)



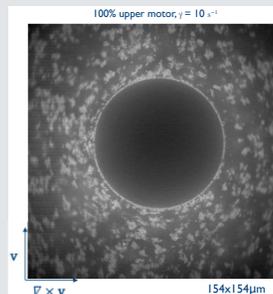
- **Brief: Method for Accelerated Aging of Dispersions**, projects submitted

- Opportunity for **computational models** in close coordination with experiments

4. Processing flows and processability

Extrusion, die slip, static zones

Complex geometries and flows



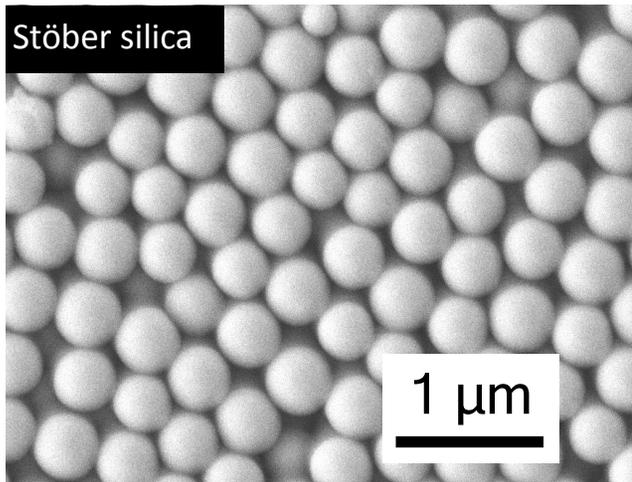
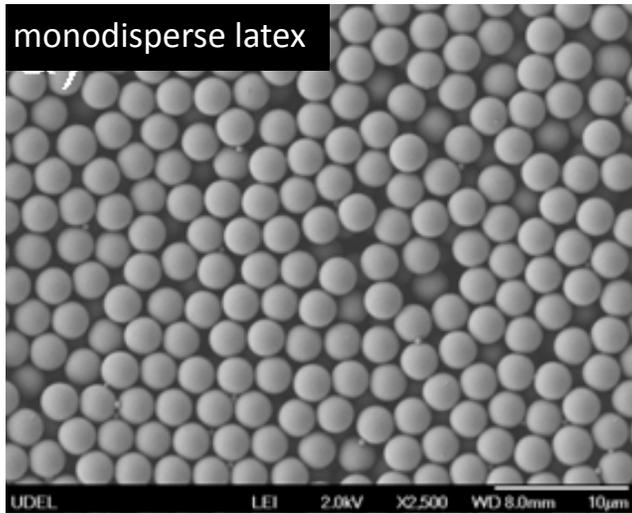
- Imaging dense suspension flows in complex geometries

- Opportunity for **computational models**

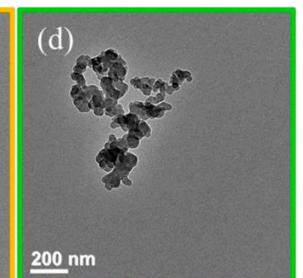
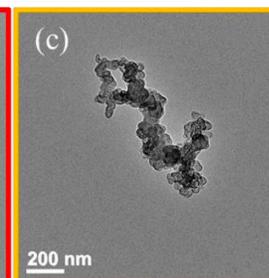
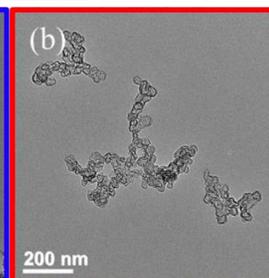
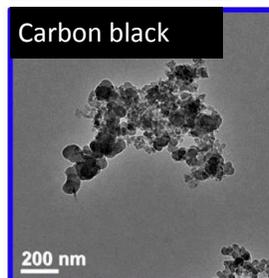
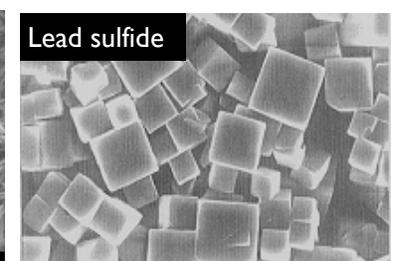
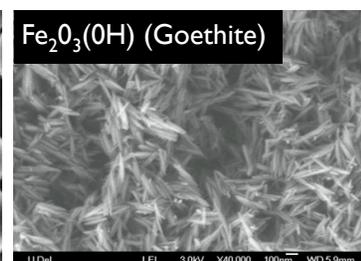
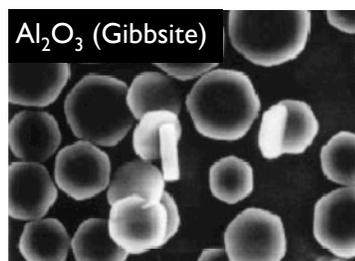
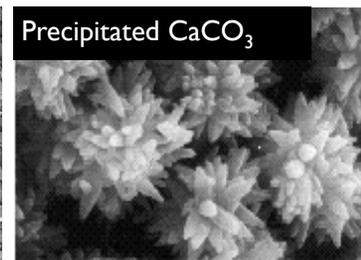
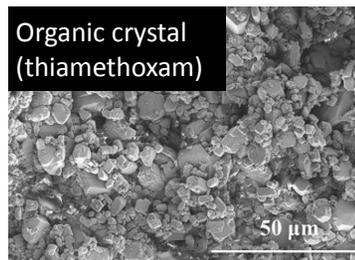
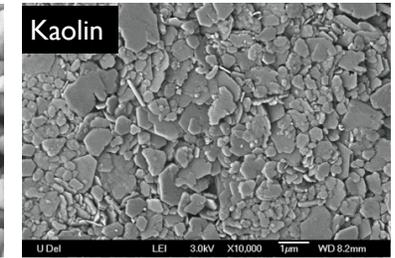
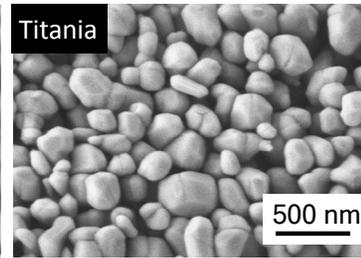
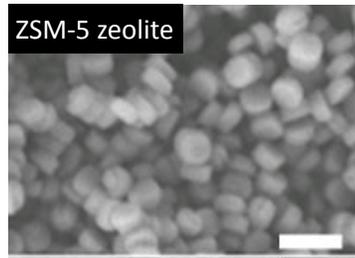
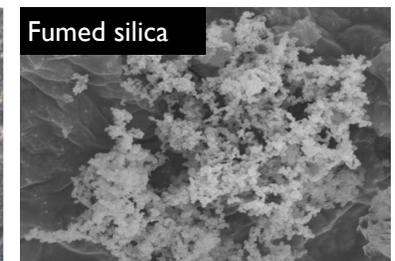
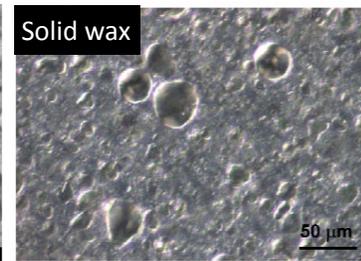
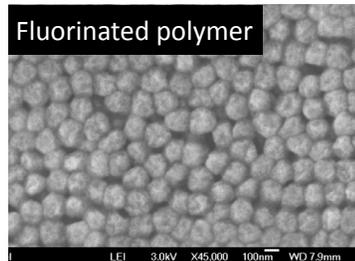
- Microstructure changes in compression (*Slurry and Paste Rheology Project*)

- ML?

Laboratory

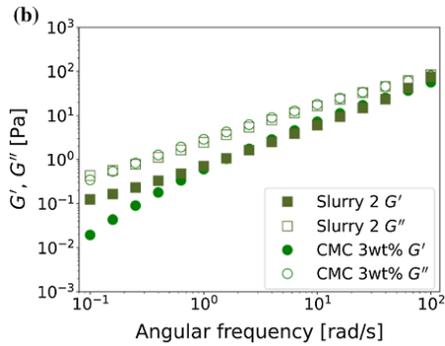
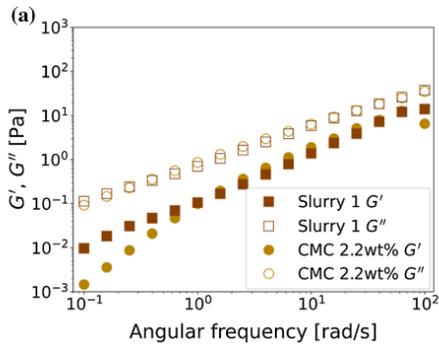
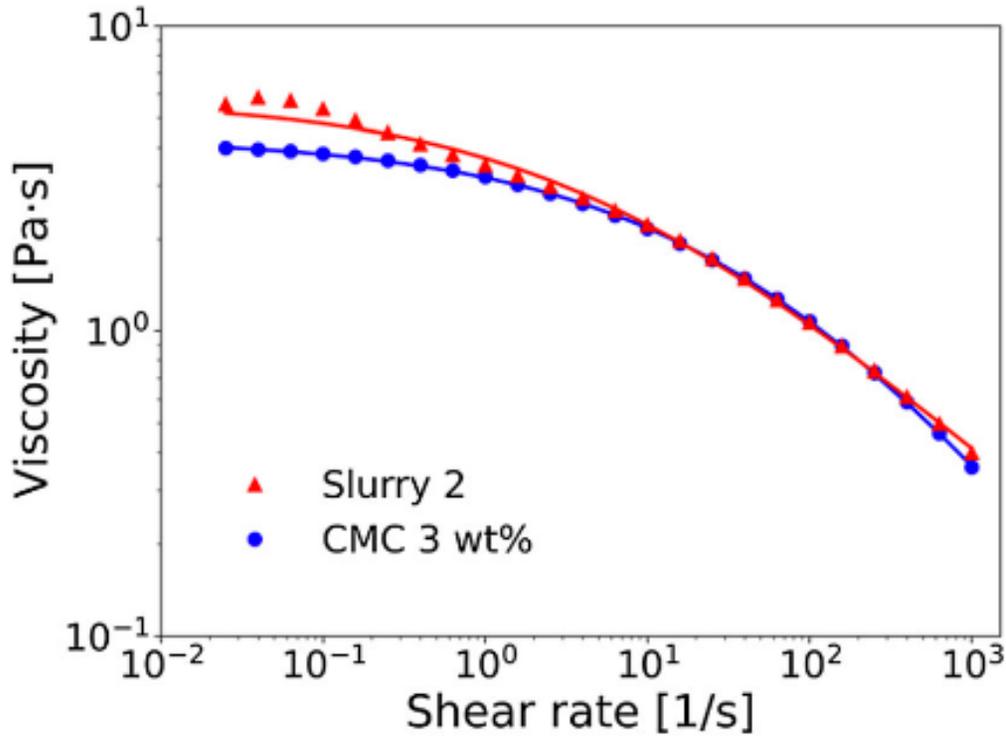


Practice



Rough / smooth
 Monodisperse / polydisperse
 Isotropic / anisotropic
 Uniform / patchy
 Prolate / oblate

Laboratory

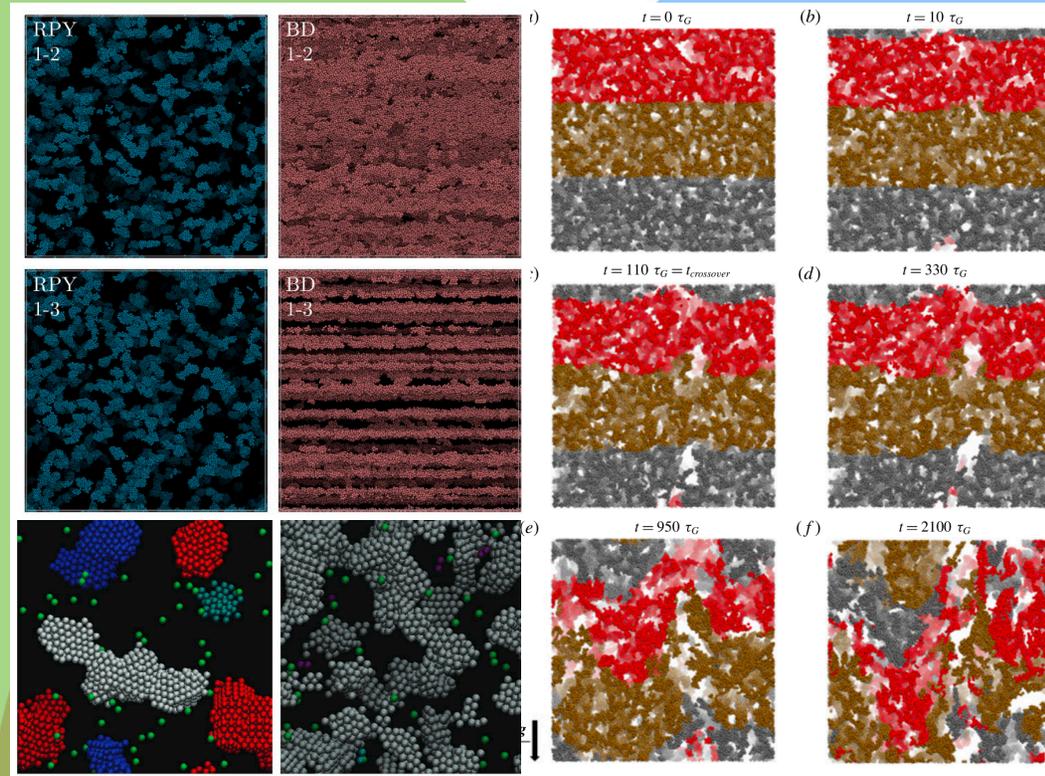


Practice



Computational modeling

Particle-scale
properties
(SIFS project)



Rheology
(SIFS, Slurry and
Paste projects)

Processing and processes
(New Accelerated Testing project)

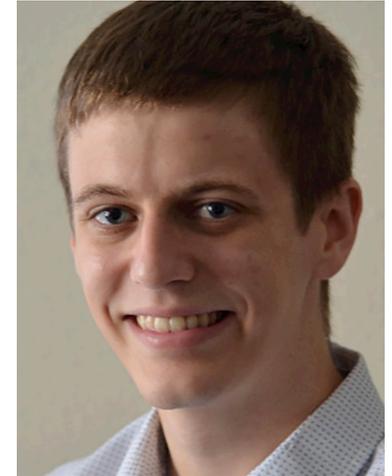
Z. Varga, J. L. Hofmann, and J. W. Swan, *J. Fluid Mech* 856, 1014 (2018).
Z. Varga and J. Swan, *Soft Matter* 79, 131 (2016).
Z. Varga, G. Wang, and J. Swan, *Soft Matter* 11, 9009 (2015).
Z. Varga and J. W. Swan, *Journal of Rheology* 62, 405 (2018).

Simulation and computational modeling

Michael Howard, Auburn University

HOOMD RPY development

- Machine learning for autonomous crystal structure identification, *Soft Matter* 13 (27), 4733-4745 2017
- Stratification dynamics in drying colloidal mixtures, *Langmuir* 33 (15), 3685-3693 2017



Zachary Sherman, University of Washington

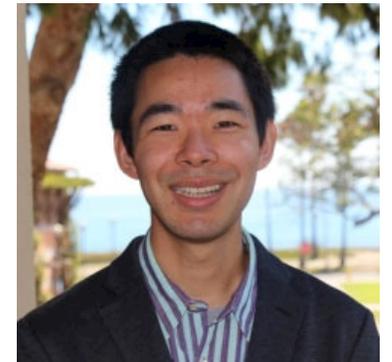
HOOMD RPY (PhD with Jim Swan), colloid assembly, colloidal gels, metamaterials

Starting fall 2023



Sho Takatori, UC Santa Barbara

Stokesian dynamics (PhD with John Brady), particle interactions, experiments / theory / simulation



Processing and characterization methods

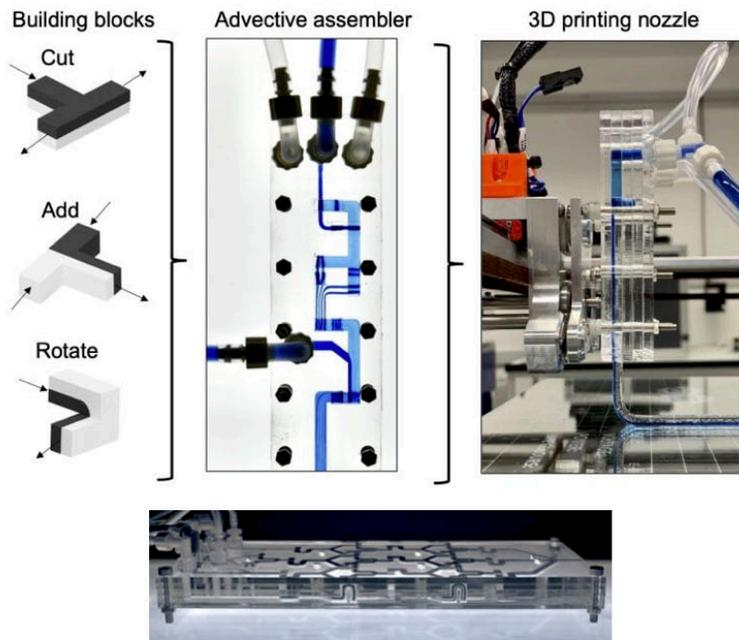
Alexandra Bayles, University of Delaware

<https://sites.udel.edu/avbayles/>

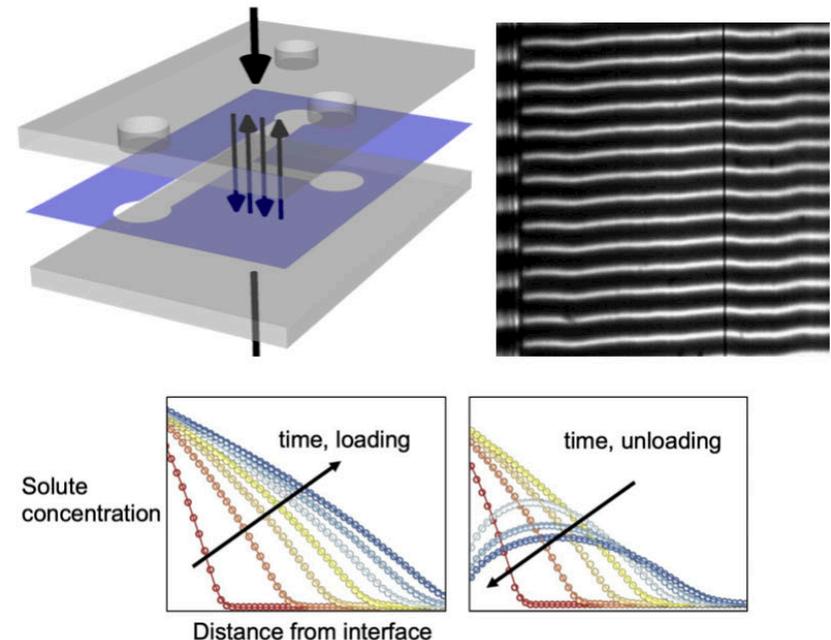
Soft materials, advective processing, microfluidic interferometry, differential dynamic microscopy, microrheology, ionic liquids and ionogels, stimuli-responsive hydrogels and emulsions



Processing and additive manufacturing



Interferometry

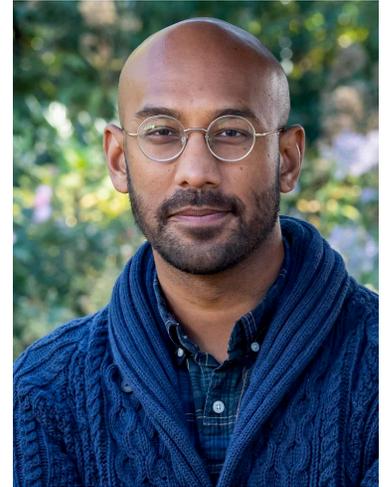


Rheology, dispersions, granular materials

Sujit Datta, Princeton University

<https://cbe.princeton.edu/people/sujit-datta>

Complex Materials and Processing, Energy and Environment



Fluid flow and deposition in porous rocks and materials

- "Multi-scale dynamics of colloidal deposition and erosion in porous media", N. Bizmark, et al., *Science Advances* 6, eabc2530 (2020)
- "Bistability in the unstable flow of polymer solutions through pore constriction arrays", C.A. Browne, et al., *Journal of Fluid Mechanics* 890, A2 (2020)

Structure, mechanics, and transport in deformable porous materials

- "Delayed buckling and guided folding of inhomogeneous capsules", S. S. Datta, et al., *Physical Review Letters* 109, 134302 (2012)
- "Crack formation and self-closing in shrinkable, granular packings", H. J. Cho, et al., *Soft Matter* 15, 4689 (2019)

Particle technology in Korea

So Youn Kim, Seoul National University

Laboratory for Soft Material Nanophysics

<https://soyounkim.snu.ac.kr/home>



Jaewook Nam, Seoul National University

Microfluidics and Coating Process Laboratory

<https://fluid.snu.ac.kr/>



EPIC – Energy & environmental materials Process integration research Center

Kyung Hyun Ahn, Seoul National University

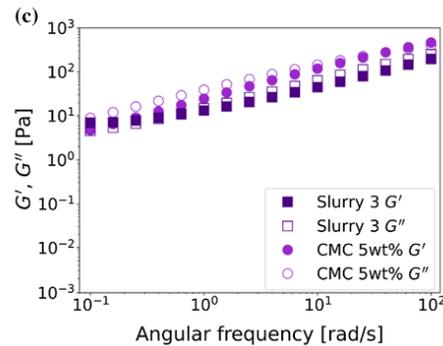
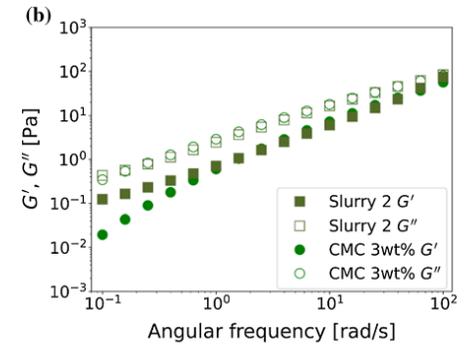
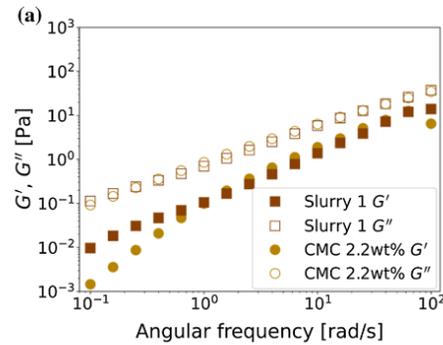
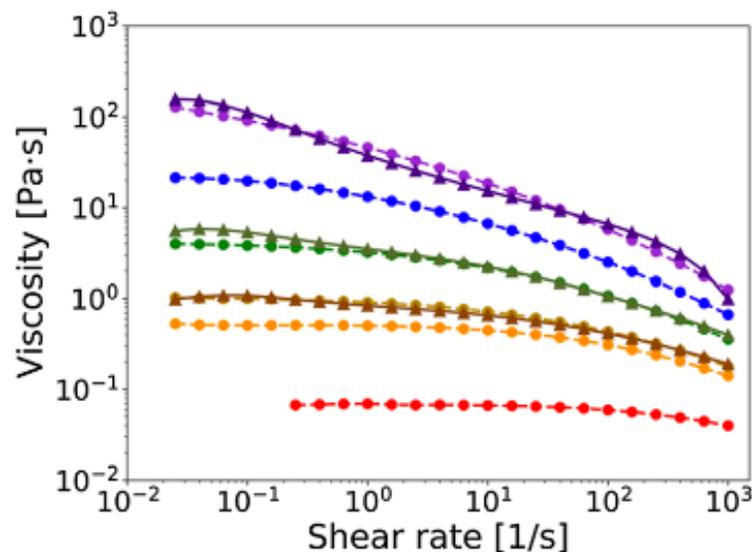
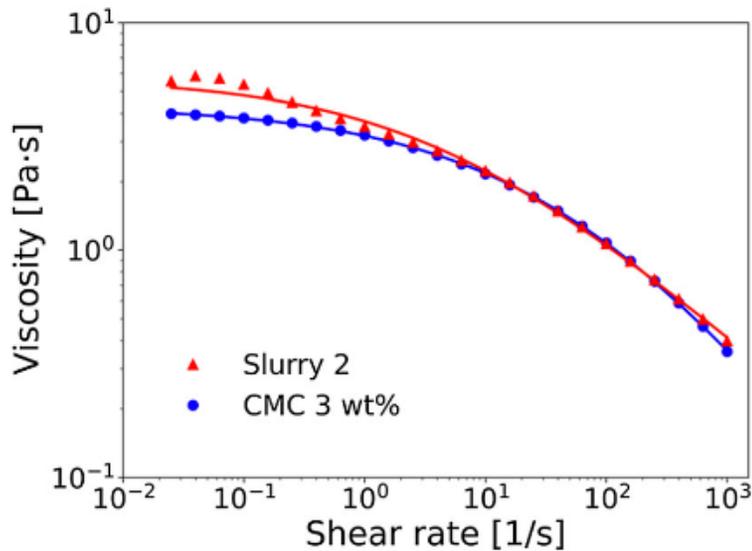
Lab for Rheology and Processing / Computational Rheology

<https://microrheology.snu.ac.kr/>



Coating Flows of Model Li-Ion Battery Anode Slurry

M. Lee, H. Jung, M. Lee, H. Kwak, and J. Nam, *J. Mater. Sci.* 57, 17935 (2022).



Anode slurries composed of graphite as the anode material, carbon black as the conductive additive, and CMC as the binder



Particle technology in Korea

Bum Jun Park, Kyung Hee University

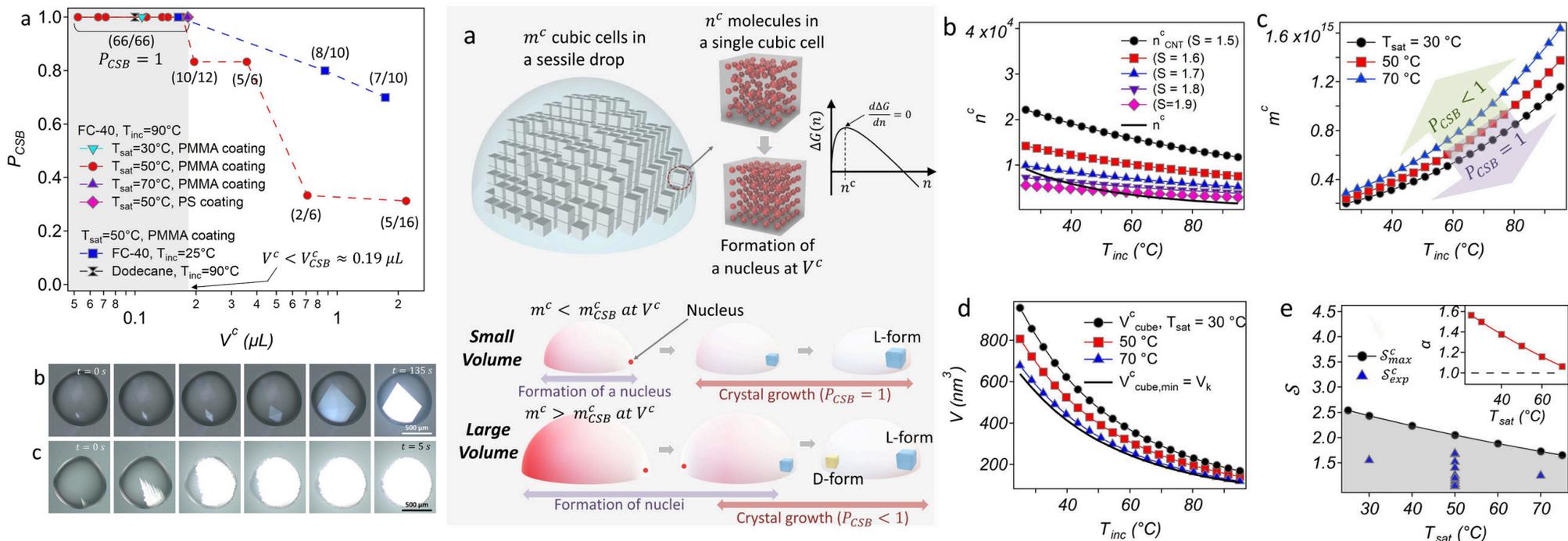
Soft Matter & Interface Engineering Laboratory

<https://www.softmatter.khu.ac.kr>



Solution Volume Effects on Spontaneous Chiral Symmetry Breaking of Sodium Chlorate Crystals

S.Y. Bak, G. Coquerel, W.-S. Kim, and B. J. Park, *J. Phys. Chem. Lett.* 14, 785 (2023).



Glasses and gels

Colloidal gels

- J. de Graaf, K. W. Torre, W. C. K. **Poon**, and M. Hermes. Hydrodynamic stability criterion for colloidal gelation under gravity. *PHYSICAL REVIEW E*, 107(3), MAR 30 2023.
- H. A. Vinutha, F. D. D. Ruiz, X. Mao, B. Chakraborty, and E. **Del Gado**. Stress-stress correlations reveal force chains in gels. *JOURNAL OF CHEMICAL PHYSICS*, 158(11), MAR 21 2023.
- *A. Clarke, E. Jamie, N. A. Burger, B. Loppinet, and G. **Petekidis**. A microstructural investigation of an industrial attractive gel at pressure and temperature. *SOFT MATTER*, 18(20):3941–3954, MAY 25 2022.
- M. Das and G. **Petekidis**. Shear induced tuning and memory effects in colloidal gels of rods and spheres. *JOURNAL OF CHEMICAL PHYSICS*, 157(23), DEC 21 2022.
- Y. Jiang, S. Makino, J. R. Royer, and W. C. K. **Poon**. Flow-switched bistability in a colloidal gel with non-brownian grains. *PHYSICAL REVIEW LETTERS*, 128(24), JUN 17 2022.
- K. Suman and N. J. **Wagner**. Anomalous rheological aging of a model thermoreversible colloidal gel following a thermal quench. *JOURNAL OF CHEMICAL PHYSICS*, 157(2), JUL 14 2022.
- L.-V. Bouthier and T. Gibaud, Three Length-Scales Colloidal Gels: The Clusters of Clusters versus the Interpenetrating Clusters Approach, *Journal of Rheology* 67, 621 (2023)
- N. Dages, L. Bouthier, V. L. Matthews, S. Manneville, T. Divoux, A. Poulesquen, and T. Gibaud. Interpenetration of fractal clusters drives elasticity in colloidal gels formed upon flow cessation. *SOFT MATTER*, 18(35):6645–6659, SEP 14 2022.
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- I. Sudreau, M. Auxois, M. Serval, E. Lecolier, S. Manneville, and T. Divoux. Residual stresses and shear-induced overaging in boehmite gels. *PHYSICAL REVIEW MATERIALS*, 6(4), APR 14 2022.

Glassy and jammed suspensions

- R. C. Roberts, J. C. Palmer, and J. C. **Conrad**. Long-wavelength fluctuations in quasi-2d supercooled liquids. *JOURNAL OF PHYSICAL CHEMISTRY B*, 127(4):961–969, FEB 2 2023.
- R. C. Roberts, J. C. Palmer, and J. C. **Conrad**. Long-wavelength fluctuations in quasi-2d supercooled liquids. *JOURNAL OF PHYSICAL CHEMISTRY B*, 2023 JAN 19 2023.
- M. Brizioli, T. Sentjabrskaja, S. U. Egelhaaf, M. Laurati, R. **Cerbino**, and F. Giavazzi. Reciprocal space study of brownian yet non-gaussian diffusion of small tracers in a hard-sphere glass. *FRONTIERS IN PHYSICS*, 10, JUN 1 2022.
- B. F. Di Dio, F. Khabaz, R. T. **Bonnecaze**, and M. Cloitre. Transient dynamics of soft particle glasses in startup shear flow. part ii: Memory and aging. *JOURNAL OF RHEOLOGY*, 66(4):717–730, JUL 2022.
- J. Song, Q. Zhang, F. de Quesada, M. H. Rizvi, J. B. Tracy, J. Ilavsky, S. Narayanan, E. **Del Gado**, R. L. Leheny, N. Holten-Andersen, and G. H. McKinley. Microscopic dynamics underlying the stress relaxation of arrested soft materials. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*, 119(30), JUL 26 2022.
- S. Zhang, E. Stanifer, V. V. Vasisht, L. Zhang, E. **Del Gado**, and X. Mao. Prestressed elasticity of amorphous solids. *PHYSICAL REVIEW RESEARCH*, 4(4), DEC 12 2022.
- A. Ghosh and K. S. Schweizer, Microscopic Activated Dynamics Theory of the Shear Rheology and Stress Overshoot in Ultradense Glass-Forming Fluids and Colloidal Suspensions, *Journal of Rheology* 67, 559 (2023).
- T. E. Kusuma, P. J. Scales, R. Buscall, D. R. Lester, and A. D. Stickland, Strain Softening of Concentrated Cohesive Particulate Suspensions Prior to Yield, 355, (2021).

Particle characteristics

Shape and patchiness

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- [30] J.-A. Ulbrich, C. Fernandez-Rico, B. Rost, J. Vialetto, L. Isa, J. S. **Urbach**, and R. P. A. Dullens. Effect of curvature on the diffusion of colloidal bananas. *PHYSICAL REVIEW E*, 107(4), APR 21 2023.
- [32] S. van Kesteren, X. Shen, M. Aldeghi, and L. **Isa**. Printing on particles: Combining two-photon nanolithography and capillary assembly to fabricate multimaterial microstructures. *ADVANCED MATERIALS*, 2023 FEB 5 2023.
- [15] L. Chambon, M. Das, E. Vasilaki, G. **Petekidis**, and M. Vamvakaki. Colloidal rod-like particles with temperature- driven tunable interactions. *LANGMUIR*, 38(45):13674–13685, NOV 15 2022.
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- [19] J. Ruiz-Franco and J. van der Gucht. Force transmission in disordered fibre networks. *FRONTIERS IN CELL AND DEVELOPMENTAL BIOLOGY*, 10, JUN 30 2022.
- [35] M. Usuelli, V. Ruzzi, S. Buzzaccaro, G. Nystroem, R. Piazza, and R. Mezzenga. Unraveling gelation kinetics, arrested dynamics and relaxation phenomena in filamentous colloids by photon correlation imaging. *SOFT MATTER*, 18(30):5632–5644, AUG 3 2022.
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Colloid friction and interactions

- A. Goyal, E. Del Gado, S. Z. Jones, and N. S. Martys. Ordered domains in sheared dense suspensions: The link to viscosity and the disruptive effect of friction. *JOURNAL OF RHEOLOGY*, 66(5):1055–1065, SEP 2022.
- F. Dragulet, A. Goyal, K. Ioannidou, R. J. M. Pellenq, and E. **Del Gado**. Ion specificity of confined ion-water structuring and nanoscale surface forces in clays. *JOURNAL OF PHYSICAL CHEMISTRY B*, 126(26):4977–4989, JUL 7 2022.
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- T. A. Prabhu and A. Singh, Rheology and Microstructure of Discontinuous Shear Thickening Suspensions, *Journal of Rheology* 66, 731 (2022).
- J. A. Ruiz-Lopez, S. S. Prasanna Kumar, A. Vazquez-Quesada, J. de Vicente, and M. Ellero, Tribological Variable-Friction Coefficient Models for the Simulation of Dense Suspensions of Rough Polydisperse Particles, *Journal of Rheology* 67, 541 (2023).
- A. Goyal, E. **Del Gado**, S. Z. Jones, and N. S. Martys, Ordered Domains in Sheared Dense Suspensions: The Link to Viscosity and the Disruptive Effect of Friction, *Journal of Rheology* 66, 1055 (2022).

Multiphase suspensions and mixtures

Colloids at interfaces

- M.-C. Tatry, E. Laurichesse, J. Vermant, V. Ravaine, and V. Schmitt. Interfacial rheology of model water-air microgels laden interfaces: Effect of cross-linking. JOURNAL OF COLLOID AND INTERFACE SCIENCE, 629(B):288–299, JAN 2023.
- A. Bayles, V and J. **Vermant**. Divide, conquer, and stabilize: Engineering strong fluid-fluid interfaces. LANGMUIR, 2022 MAY 18 2022.
- *A. Czakaj, E. Chatzigiannakis, J. **Vermant**, M. Krzan, and P. Warszynski. The influence of the surface chemistry of cellulose nanocrystals on ethyl lauroyl arginate foam stability. POLYMERS, 14(24), DEC 2022.
- *J. Vialetto, S. N. Ramakrishna, and L. **Isa**. In situ imaging of the three-dimensional shape of soft responsive particles at fluid interfaces by atomic force microscopy. SCIENCE ADVANCES, 8(45), NOV 11 2022.
- M. E. A. Zakhari and R. T. **Bonnecaze**. Slip-stick transitions of soft permeable particles near a repulsive wall. SOFT MATTER, 18(22):4239–4252, JUN 8 2022.

Deposition and porous media

- D. Mangal, J. C. **Conrad**, and J. C. Palmer. Nanoparticle dispersion in porous media: Effects of attractive particle-media interactions. PHYSICAL REVIEW E, 105(5), MAY 10 2022.
- T. Shende, D. Mangal, J. C. Conrad, V. Niasar, and M. Babaei. Nanoparticle transport within non-newtonian fluid flow in porous media. PHYSICAL REVIEW E, 106(1), JUL 11 2022.

Capillary suspensions and drying

- *J. Allard, S. Burgers, M. C. R. Gonzalez, Y. Zhu, S. De Feyter, and E. **Koos**. Effects of particle roughness on the rheology and structure of capillary suspensions. COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS, 648, SEP 5 2022.
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Colloid polymer mixtures

- D. Parisi, D. Truzzolillo, A. H. Slim, P. Dieudonne-George, S. Narayanan, J. C. **Conrad**, V. D. Deepak, M. Gauthier, and D. Vlassopoulos. Gelation and re-entrance in mixtures of soft colloids and linear polymers of equal size. MACROMOLECULES, 56(5):1818–1827, MAR 14 2023.
- G. Legrand, S. Manneville, G. H. McKinley, and T. Divoux. Dual origin of viscoelasticity in polymer-carbon black hydrogels: A and electrical. MACROMOLECULES, 56(6):2298–2308, MAR 28 2023.
- G. Legrand, S. Manneville, G. H. McKinley, and T. Divoux. Dual origin of viscoelasticity in polymer-carbon black hydrogels: A rheometry and electrical spectroscopy study. MACROMOLECULES, 2023 MAR 14 2023.
- *M. J. J. Gallegos, D. D. D. Soetrisno, N. Park, and J. C. C. **Conrad**. Aggregation and gelation in a tunable aqueous colloid-polymer bridging system. JOURNAL OF CHEMICAL PHYSICS, 157(11), SEP 21 2022.
- ***M. A. A. Joens, P. S. S. Doyle, G. H. H. McKinley, and J. W. W. **Swan**. Time-dependent two-dimensional translation of a freely rotating sphere in a viscoelastic fluid. PHYSICS OF FLUIDS, 34(12), DEC 2022.
- F. S. Samghabadi, A. H. Slim, M. W. Smith, M. Chabi, and J. C. **Conrad**. Dynamics of filamentous viruses in polyelectrolyte solutions. MACROMOLECULES, 55(23):10694–10702, DEC 13 2022.

Processing rheology

Thixotropy

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IFPRI Wet Systems Investigators



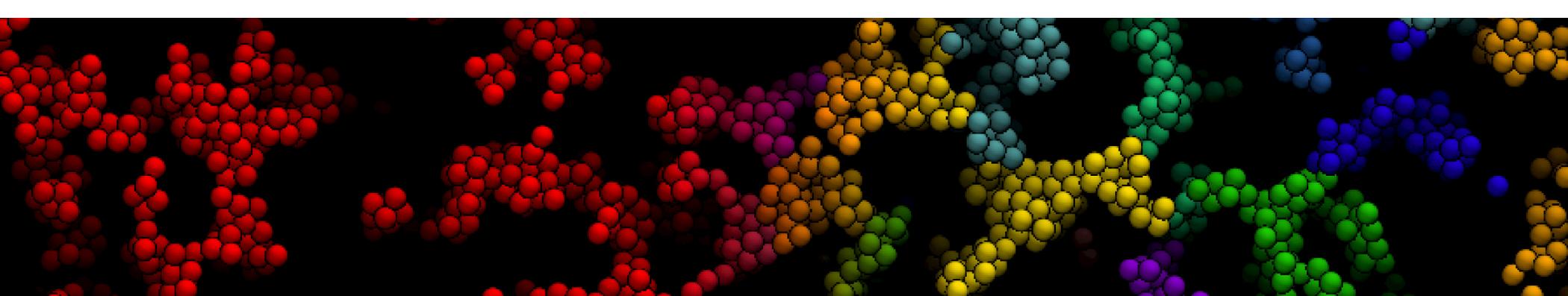
PI	Institution	Research portfolio	IFPRI engagement	website
Lilian Hsiao*	North Carolina State University, Chemical and Biomolecular Engineering	Shaped colloids and functionalized surfaces	Active IFPRI collaboration with Vermont, 2019 proposal	http://www.hsiaolab.com
Lucio Isa*	ETH, Zürich, Materials	Colloid friction / tribology	Collaborator with Vermont / SIF project	https://isa.mat.ethz.ch
Roger Bonnezaze	UT Austin, Chemical Engineering	Computational modeling, theory	2018 Report	https://sites.utexas.edu/bonnezazegroup/
Emanuela Del Gado	Georgetown, Physics	Modeling and theory of suspensions	None	http://delgadolab.georgetown.domains
Jeff Morris	City College of New York, Levich Institute	Computational modeling, theory	None	https://levich.ccny.cuny.edu/morris-laboratory/
Xavier Chateau	Université Paris-Est / École des Ponts	Pastes, cements, contact mechanics	None	https://navier-lab.fr/en/equipe/chateau-xavier/
Guillaume Ovarlez	Université de Bordeaux	Rheology, shear thickening, non-Brownian suspensions	None	https://www.lof.cnrs.fr/guillaume-ovarlez/
Ron Larson	Michigan	Rheology, computational modeling, 2019 thixotropy review	None	http://cheresearch.engin.umich.edu/larson/
Dan Blair & Jeff Urbach	Georgetown, Physics	Friction and jamming in dense suspensions, spatio-temporal cross-correlation	2018 proposal not selected (Blair)	https://blairlab.georgetown.edu

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PI	Institution	Research portfolio	IFPRI engagement	website
Jaci Conrad	University of Houston, Chemical Engineering	Colloids in confinement and in flow	None	https://www.chee.uh.edu/faculty/conrad
Randy Ewoldt	Illinois Urbana-Champaign, Mechanical Engineering	Non-Newtonian fluid mech, non-linear rheology, yield stress fluids	None	https://ewoldt.mechanical.illinois.edu
Frank Scheffold	University of Fribourg, Physics	Light scattering, dense suspensions and emulsions	None	https://www.unifr.ch/phys/en/research/groups/scheffold/
Roberto Cerbino	University of Vienna	Differential dynamic microscopy, suspension dynamics	None	https://sites.google.com/site/cerbino/
Patrick Anderson	TU Eindhoven	Computational / Applied rheology and process modeling	None	https://scholar.google.com/citations?user=m-Q4RrAAAAAJ&hl=en&oi=ao
Peter Schall	Amsterdam, Physics	Glasses and yielding, nanomechanics, particle interactions	None	https://peterschall.de
Luca Cipelletti	University Montpellier	Jamming, glasses, light scattering	None	https://coulomb.umontpellier.fr/user/luca.cipelletti
Roberto Piazza	Politecnico di Milano	Colloidal gels and glasses	None	https://scholar.google.com/citations?user=IGnqIMYAAAAAJ&hl=en&oi=ao
Vinny Manoharan	Harvard	Holographic microscopy of dispersions	None	https://manoharan.seas.harvard.edu
Alex Routh	Cambridge	Film Formation and dispersion drying, Aggregation	None	https://www.ceb.cam.ac.uk/directory/alex-routh

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PI	Institution	Research portfolio	IFPRI engagement	website
Jasper Van der Gucht	Wageningen University	Networks, contact networks	None	https://www.wur.nl/en/Research-Results/Chair-groups/Agrotechnology-and-Food-Sciences/Physical-Chemistry-and-Soft-Physics
George Petekidis	University of Crete / FORTH	Dense suspension rheology	2019 proposal not selected	https://www.iesl.forth.gr/en/people/petekidis-george
Joost de Graaf	Institute for Theoretical Physics, Utrecht	Dense suspension rheology	None but collaborating with Kool	https://webpace.science.uu.nl/~graaf156/group.html



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