2026 Helmholtz – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Process-Oriented Computer Simulation of Morphology Formation in Printed Photovoltaics and Printed Electronics

Helmholtz Centre and/or institute:

Forschungszentrum Jülich GmbH,
Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IET-2)

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Dynamics of Complex Fluids and Interfaces

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Description of the project (max. 1 page)**:**

Organic photovoltaic (OPV) devices present attractive properties (e.g., light weight, flexibility, semi-transparency, tunable colors, discretionary shapes, etc.) that extend photovoltaic applications beyond traditional silicon solar panels. However, reliable commercialization remains challenging, in particular due to the need for robust, scalable manufacturing based on solution-deposition techniques such as inkjet printing. These challenges are emblematic of the broader field of printed electronics, which aims at low-cost, large-area fabrication of functional devices on flexible substrates. Achieving industrial relevance therefore requires precise control over ink formulation, printing processes, and post-deposition treatments to ensure device performance and reproducibility. In this context, controlling the nanomorphology of printed active layers, which constitute the functional core of OPV and other printed electronics devices, is of central importance. However, the mechanisms governing the emergence of nanomorphological features during processing remain insufficiently understood. Consequently, integrated theoretical and experimental approaches are required, as they enable a deeper insight into the physical processes underlying active-layer nanostructure formation and provide a rational basis for process optimization.

The two-year postdoctoral project splits into two parts, with the objectives to improve our understanding of active layer morphology formation during inkjet printing of organic solar cells and to develop new deposition processes based on capillary-force driven self-assembly of nanoparticles.

In the first part, a recently developed phase-field simulation framework will be employed to study active-layer morphology formation during inkjet printing of organic solar cells. Inkjet-printed active layers are typically formed by the successive deposition of partially overlapping stripes of photoactive ink, where newly deposited material interacts with regions that have already undergone partial solvent evaporation and structural evolution. This work package aims at the simulation of the coupled processes governing morphology development in this scenario, including solvent evaporation, fluid flow, phase separation, remixing, and crystallization. Particular emphasis is placed on elucidating how the solvent and material composition of a newly deposited stripe influence the stability and evolution of pre-existing nanostructures in the underlying layer. In a subsequent step, the postdoctoral researcher will investigate the aggregation behavior of non-fullerene acceptors (NFA) in binary OPV blends as a function of concentration. Depending on the blend ratio with polymer donors, NFAs exhibit distinct aggregation regimes that critically influence device performance. Experimental characterization of these aggregation processes performed by our collaborators at the Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO) will be systematically compared with phase-field simulations of nanostructure formation.

The second part of the project focuses on developing a systematic theoretical and numerical framework to understand and control nanoparticle assembly guided by liquid bridges, with the goal of enabling the rational design of three-dimensional architectures for printable electronics. Capillary bridges provide confinement and controlled dewetting, enabling precise particle stacking and patterning; however, despite experimental demonstrations, a comprehensive theoretical description of liquid-bridge-guided assembly remains lacking. In particular, the coupled dynamics of meniscus evolution and particle motion, as well as the influence of the particle properties (e.g., size, shape, and wettability), are not yet fully understood. The postdoctoral researcher will establish a quantitative, continuum-level theoretical description of liquid bridge formation and evolution during evaporation between. This model will be validated using multicomponent/multiphase lattice Boltzmann simulations. Then, a particle-resolved, coupled lattice Boltzmann and discrete element method will be employed to simulate the fluid-particle system. The influence of key particle properties—including size, shape, interparticle interactions, and wettability—as well as the particle-substrate interactions will be systematically studied. The simulation results will be compared with experimental data from our collaborators at SINANO. Ultimately, we seek to identify conditions under which capillary bridges enable controlled outcomes—such as directional alignment, bundling, or network formation—that are critical for applications in printed and flexible electronics.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

We maintain an active research collaboration with Prof. Chang-Qi Ma at the Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO), Chinese Academy of Sciences, China. Prof. Ma leads the i-Lab and the Printable Electronics Research Centre at SINANO. The collaboration focuses on the nanomorphological properties of printed organic photoactive layers and the assembly and alignment of nanowires for flexible electronic devices. Prof. Ma's group possesses strong experimental expertise in printable flexible electronics and thin-film solar cells. Our group provides complementary theoretical modeling and numerical simulation expertise, aimed at elucidating the underlying fundamental material- and process- properties governing the printing of flexible electronics and organic photovoltaic devices.

This synergistic experimental–theoretical collaboration has recently led to the acceptance of a joint research article for publication in the journal Droplet, highlighting the effectiveness of our combined approach.

Institute website of SINANO
http://english.sinano.cas.cn/

Prof. Chang-Qi Ma
Email: cqma2011@sinano.ac.cn
Personal webpage:
http://english.sinano.cas.cn/sourcedb/people/faculty/201110/t20111019_378767.html

Required qualification of the postdoc:

- PhD in Physics, Computational Science, Chemical Engineering, Materials Science, or a closely related discipline.
- Experience in numerical modeling and simulations, with demonstrated expertise in soft matter systems such as colloids, polymers, or complex fluids.
- Additional skills in scientific programming and data analysis, with practical experience in Python/Matlab/Fortran/C++ et al.; familiarity with high-performance computing environments is an advantage.
- Language requirement: excellent communication skills, including fluency in written and spoken English.