Beitrag ID: **47** Typ: **Talk**

# Volatile binary mixtures on polymer brushes

*Dienstag, 5. Dezember 2023 10:10 (25 Minuten)*

We present a mesoscopic thin-film model in gradient dynamics form for binary liquid mixtures on brush-covered substrates incorporating volatility in a narrow gap. Thereby, we expand models established in [1, 3, 4], for one substance by incorporating a second substance present in each of the three bulk phases - liquid, brush and gas [1, 2]. We discuss the different contributions to the free energy, thereby employing Flory-Huggins theory of mixing for the condensed phases and assuming ideal gases for the vapor phase. Interface energies are modeled as linear interpolations of known limiting cases. The resulting six-field model is then analyzed with numerical time simulations showing results with a focus on lateral concentration gradients, notably at the contact line.

[1] S. Hartmann, C. Diddens, M. Jalaal, and U. Thiele. Sessile drop evaporation in a gapcrossover between diffusion-limited and phase transition-limited regime. June 2022.
[2] L. A. Smook, G. C. R. van Eck, and S. de Beer. Friends, foes, and favorites: Relative interactions determine how polymer brushes absorb vapors of binary solvents. Macromolecules, 53(24):10898–10906, dec 2020. doi: 10.1021/acs.macromol.0c02228.
[3] U. Thiele and S. Hartmann. Gradient dynamics model for drops spreading on polymer brushes. The European Physical Journal Special Topics, 229(10):1819–1832, sep 2020. doi: 10.1140/epjst/e2020-900231-2.
[4] ¨Ozlem Kap, S. Hartmann, H. Hoek, S. de Beer, I. Siretanu, U. Thiele, and F. Mugele. Nonequilibrium configurations of swelling polymer brush layers induced by spreading drops of weakly volatile oil. The Journal of Chemical Physics, 158(17), 2023. doi: 10.1063/5.0146779

**Hauptautoren:** DIEKMANN, Jan; THIELE, Uwe

**Vortragende(r):** DIEKMANN, Jan

**Sitzung Einordnung:** Short Talks