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Molecular Dynamics Study of Self-propelled Droplets on Solid Substrates MURAT MÜLAYIM, MARCUS MÜLLER, Georg-August Universität — We study, by molecular simulation, the statics and dynamics of chemically driven polymer droplets on regularly and finely corrugated substrates. Droplets are driven by a self-induced wettability gradient, which is formed under the droplet by changing the strength of the polymer-substrate interaction when the polymer get into contact with a reactive substrate with a pre-defined probability. The effect of reaction rate on droplet profile, slip and motion are investigated in the quasi steady-state. Moreover wetting properties of heterogeneous, partially reacted, systems are studied and a connection to experiments in the literature and thin film theoretical results on driven droplets are drawn, via exploring velocity profiles and dissipation mechanisms in the system.

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