Wetting and Recovery of Nano-Patterned Surfaces Beyond the Classical Picture

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August 20, 2019

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Figure SI1: Logarithmm of the joint probability density function $\rho(\Delta N, N)$ along reactive trajectories in the system with the 20 × 20 pore at pressures P = -0.005 (A) and P = 0.035 (B). With increasing pressure the intrusion mechanism passes from asymmetric (A) to symmetric (B).



Figure SI2: Pairs of $(\Delta N, N)$ values sampled in RMD simulations of the wetting/recovery process at P = 0.035, 0.01, -0.005, -0.08 and -0.168. The dashed lines, introduced to help the reader to follow the wetting/recovery path, is obtained by connecting the average value of ΔN at each N, $\langle \Delta N \rangle_N$; in the region in which the graph is split in the two parts $(N > 450) \langle \Delta N \rangle_N$ is computed within the domain of each mode. Independently on the pressure, in the early part of the wetting ΔN values are concentrated about 0. At $N \sim 450$ one observes a sharp change, with sizably negative and positive ΔN values. The recovery path is just the opposite of the wetting one.



Figure SI3: Duration of reactive trajevvtories Δt vs liquid pressure P in LJ units. These results show that the increase of the wetting and recovery driving force, increase and decrease of the liquid pressure, respectively, shorten the duration of reactive trajectories. Nevertheless, the variation of the duration of reactive trajectories, which change of a factor 2 - 3, is much shorter than the variation of the transition time τ , which changes of 27 orders of magnitude. Indeed, as explained in the main text, the origin of the variation of the transition time is not the duration of reactive trajectories but the frequency with which attemped transition from the Cassie-Baxter to the Wenzel state and vice versa are successful.