

In terms of the project on 'Active Drying', we discussed the initial stages. 'Drying' is an equilibrium surface phase transition that occurs when a fluid at liquid-vapour coexistence is in contact with an infinite planar substrate that is sufficiently weakly attractive to the fluid particles, such that the vapour phase prefers to be at the substrate. Surface phase transitions can be first-order or critical, and previous results (see attached paper by Evans et al.) show that drying is generally a critical surface phase transition.

Previous work on ABPs has shown that they can exhibit a first-order wetting transition (see Turci et al., attached). This effect has been investigated by looking at liquid-vapour 'slabs' and droplets, showing consistent results. However, the mechanism by which the wetting transition is traversed does not seem to allow for the possibility of a drying transition. To have a chance of observing this, we need to understand the mechanism by which ABPs interact with a surface.

The aggregation effect at a hard wall arises because ABPs become trapped at the wall and cannot diffuse away quickly enough. The project will attempt to induce a drying transition by coupling the ABP velocity vector to the wall-fluid interaction in such a way as to produce a torque that creates an effective wall-fluid repulsion, possibly enabling a drying transition. Your task will be to modify a standard MD simulation package to introduce this torque and then proceed similarly to the Turci and Wilding paper in *PRL* 2021, to try to observe a drying transition. If evidence for this is seen, then you will try to quantify the character of the transition and analyse its critical properties.

In terms of the project on 'Active Drying', we discussed the initial stages. 'Drying' is an equilibrium surface phase transition that occurs when a fluid at liquid-vapour coexistence is in contact with an infinite planar substrate that is sufficiently weakly attractive to the fluid particles, such that the vapour phase prefers to be at the substrate. Surface phase transitions can be first-order or critical, and previous results (see attached paper by Evans et al.) show that drying is generally a critical surface phase transition.

Previous work on ABPs has shown that they can exhibit a first-order wetting transition (see Turci et al., attached). This effect has been investigated by looking at liquid-vapour 'slabs' and droplets, showing consistent results. However, the mechanism by which the wetting transition is traversed does not seem to allow for the possibility of a drying transition. To have a chance of observing this, we need to understand the mechanism by which ABPs interact with a surface.

The aggregation effect at a hard wall arises because ABPs become trapped at the wall and cannot diffuse away quickly enough. The project will attempt to induce a drying transition by coupling the ABP velocity vector to the wall-fluid interaction in such a way as to produce a torque that creates an effective wall-fluid repulsion, possibly enabling a drying transition. Your task will be to modify a standard MD simulation package to introduce this torque and then proceed similarly to the Turci and Wilding paper in *PRL* 2021, to try to observe a drying transition. If evidence for this is seen, then you will try to quantify the character of the transition and analyse its critical properties.