Supporting information for: Dynamical Insights into the Mechanism of a Droplet Detachment from a Fiber

Neda Ojaghlou [a], Hooman V. Tafreshi [b], D. Bratko [a,*], and Alenka Luzar [a,*]

[a] Department of Chemistry, Virginia Commonwealth University, Richmond, Virginia 23284, United States

[b] Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, Virginia 23284, United States

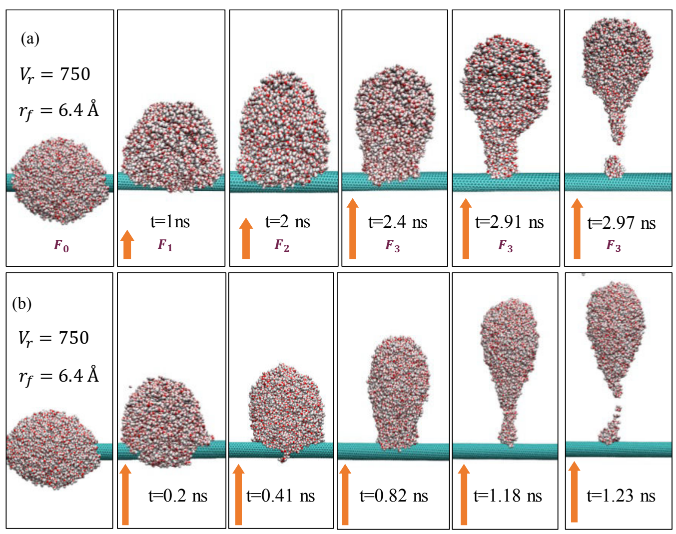

Figure S1. Snapshots from a MD trajectory during the droplet detachment from a fiber for the atomistic model with $V_r = 750$ and fiber radius $r_f = 6.4$ Å. (1-a): snapshots at different times t and corresponding external forces F_o=0, F_1=0.0041, F_2=0.0046, and F_3=0.005 $kJ\ mol^{-1}$Å^{-1}. The force is increased gradually until the drop is about to detach from the fiber. (1-b): snapshots showing the evolution of droplet shape at constant force, F=0.0058 $kJ\ mol^{-1}$Å^{-1}, exerted on the droplet during the simulation.

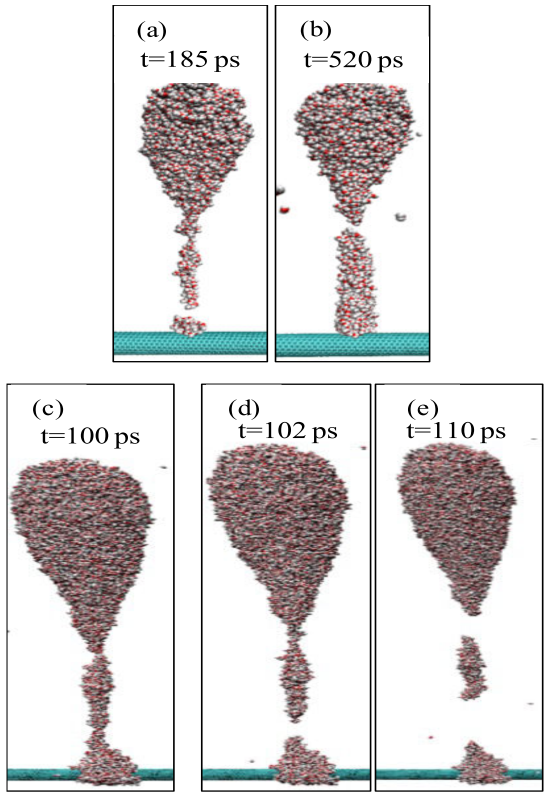

Figure S2. Snapshots from MD trajectories of the droplet detachment from a fiber for the atomistic model. Figures a-b show that the breakup takes place at different distances from the fiber and different times during two different atomistic simulation run s with $V_r = 500$. The droplet consists of 4000 SPC/E water molecules and the fiber radius is 6.4 Å. The force is F=0.0125 $kJ\ mol^{-1}Å^{-1}$. Figures c-e show the formation of a satellite droplet following the detachment of the drop from the fiber under the force F=0.0292 $kJ\ mol^{-1}Å^{-1}$ for the atomistic water model and $V_r = 2000$. The droplet contains 17000 SPC/E water molecules and the fiber radius $r_f = 6.4$ Å.