Functionalized carbon nanocones as a water harvesting device.

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In the work we investigate through molecular dynamic simulations the water capture process for functionalized carbon nanocones (CNC) in three scenarios: a single CNC in contact with a reservoir containing liquid water, a single CNC in contact with water vapor reservoir and a combination of more than one CNC also in contact with vapor. We found that water flows through the nanocones when in contact with the liquid reservoir if nanocone tip presents hydrophilic functionalization. In contact with steam, we observed the formation of droplets at the base of the nanocone only when hydrophilic functionalization is present. Then, water flows through a linear in a process that is more efficient than in the liquid reservoir regime. Varying hydrophilicity, we found an optimum value of attraction that maximizes water capture from the vapor. The scalability of the process is tested by analyzing the water flow through more than one nanocone. The results suggest that the distance between the nanocones is a fundamental ingredient for the efficiency of the water harvesting. This work was published in two articles [1][2]. Also, an experimental study was conducted to analyze the transport properties of an alumina membrane with nanocones, modified to alter wettability, under varying humidity levels [3].

References

[1] Leivas, F. R.; Barbosa, M. C. Beilstein J. Nanotechnol. 2023, 14, 1–10. doi:10.3762/bjnano.14.1

[2] F. R. Leivas and M. C.Barbosa; J. Chem. Phys. 15 May 2023; 158 (19): 194702.

[3] Leivas, F. R.; Biance, A. L.; Canut, S. R.; Bizzone C. C.; Barbosa, M. C. ; “Condensation effect and transport on Al porous membranes” Langmuir.

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