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Molecular Dynamics Simulations of Fluorinated Bottlebrush Copolymers in Thin Films[1] JAN-MICHAEL CARRILLO, DONGSOOK CHANG, KUNLUN HONG, BOBBY SUMPTER, Oak Ridge National Laboratory
— We have performed multi-scale molecular dynamics (MD) simulations of bottlebrush copolymers with fluorinated side-chains. In thin films, coarse-grained MD simulations reveal that side-chains are preferentially located at interfaces and are slightly oriented perpendicular to the interface. At the molecular level, atomistic MD simulations show that fluorine atoms in the bottlebrush are preferentially located at interfaces, as well. Both simulation results indicate enhancement of fluorinated moieties at interfaces providing a probable explanation to the increase in hydrophobicity of the spin-coated thin films from these bottlebrush copolymers.

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