Atomistic simulations of processes in acrylic paints

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We performed fully atomistic models of two types of acrylic paints to understand their structure and interaction with volatile organic compounds (VOCs) and water. The structure and properties of acrylic copolymers are slightly modified by incorporation of a monomer with a longer side chain. With favorable solvation free energies, once absorbed, VOCs and water interact with the polymer side chains to form hydrogen bonds. The cage like structure of the polymers prevents the VOCs and water to diffuse freely below the glass transition temperature. In addition, we use these simulations for developing mesoscopic models and to study initial degradation processes.

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