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Molecular dynamics of reversible self-healing materials IAN MADDEN, ERIK LUIJTEN, Northwestern University — Hydrolyzable polymers have numerous industrial applications as degradable materials. Recent experimental work by Cheng and co-workers (*Nat. Comm.* **5**, 3218 (2014)) has introduced the concept of hindered urea bond (HUB) chemistry to design self-healing systems. Important control parameters are the steric hindrance of the HUB structures, which is used to tune the hydrolytic degradation kinetics, and their density. We employ molecular dynamics simulations of polymeric interfaces to systematically explore the role of these properties in a coarse-grained model, and make direct comparison to experimental data. Our model provides direct insight into the self-healing process, permitting optimization of the control parameters.

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