Winter 2025 Joint Colloquium Materials Department & Materials Research Laboratory

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Self-assembly models for crystal growth and phase transitions

How can we make new materials and better understand how their underlying structures form? The direct observation of crystal growth and transitions remains supremely challenging, but gaining insight into these fundamental processes is central to our quest of creating materials in a rational and targeted way, connecting structure to functionality. We build self-assembly models, study how they react to perturbations on the particle and system levels, and investigate their impact on crystal growth and transformation pathways. We use simple coarse-grained models to gain systematic insights into the phenomena that lead to the crystallization of complex crystal structures, partial disorder, or magic-size assemblies, allowing us to derive the essential principles that govern the formation of materials' structures. Our goal is to use these insights to find ways to tailor crystallization pathways and to create new functional materials. Our work promises to establish new pathways to materials design through simulations, which explicitly incorporate and explore phase transformation kinetics.

Hosted by Raphaele Clement