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ABSTRACT

Functional glasses play a critical role in current and developing technologies. These materials have traditionally been designed empirically through trial-and-error experimentation. However, here we report recent advancements in the design of new glass compositions starting at the atomic level, which have become possible through an unprecedented level of understanding of glass physics and chemistry. For example, new damage-resistant glasses have been developed using models that predict both manufacturing-related attributes (e.g., viscosity, liquidus temperature, and refractory compatibility), as well as the relevant end-use properties of the glass (e.g., elastic moduli, compressive stress, and damage resistance). We demonstrate how this approach can be used to accelerate the design of new industrial glasses for use in various applications. Through a combination of models at different scales, from atomistic through empirical modeling, it is now possible to decode the "glassy genome" and efficiently design optimized glass compositions for production at an industrial scale.