Decoding the Structural Genome of Silicate Glasses

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Silicate glasses can exhibit a wide range of properties. To understand, tune, and enhance glasses' properties, one needs to decode the "glass genome," that is, to uncover how basic structural features control glass' macroscopic properties—in the same fashion as DNA governs a given individual's characteristics. This requires as a prerequisite the accurate knowledge of the atomic structure of silicate glasses. However, experiments typically offer indirect signatures of the three-dimensional atomic structure of glasses (e.g., coordination numbers, pair distribution functions). On the other hand, although molecular dynamics (MD) simulations offer direct access to glasses' structure, they come with their own shortcomings (e.g., very high cooling rates). Here, we present force-enhanced atomic refinement (FEAR) as a powerful modeling technique to unveil the three-dimensional structure of glasses. We demonstrate that FEAR yields glass structures that simultaneously exhibit improved thermodynamic stability as compared to MD, but also an unmatched level of agreement with experimental data. We show how the use of FEAR allows us to solve several puzzles in glass science, including how the atomic structure of glasses governs their response to changes in temperature and pressure.