# Topological control on glasses' dissolution kinetics

Mathieu Bauchy*†[1] and Morten Smedskjær[2]

[1]University of California, Los Angeles (UCLA) – United States
[2]Aalborg University – Denmark

**Abstract**

Understanding and predicting the dissolution rate of silicate glasses is of primary importance for various applications, including bioactive glasses and borosilicate wasteforms. However, the mechanism of silicates' dissolution-and its rate-limiting step-remains poorly understood. In particular, present models linking the composition and structure of silicate glasses to their dissolution rate in a given solvent have remained largely empirical thus far. Here, based on vertical scanning interferometry (VSI) experiments and molecular dynamics (MD) simulations, we study the dissolution of a large variety of silicate glasses under various pH conditions. From a detailed analysis of the simulated structures, we demonstrate that the kinetics of the dissolution is controlled by the topology of the atomic network. We propose a new topological model of silicates' corrosion, which is shown to offer realistic predictions of dissolution rates and activation energies for a wide selection range of silicate glasses and crystals.

**Keywords:** Dissolution, Topological constraint theory, Molecular Dynamics

*Speaker
†Corresponding author: bauchy@ucla.edu