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Wang, Mengyi; Smedskjær, Morten Mattrup; Mauro, John C.; Bauchy, Mathieu

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A New Transferable Inter-Atomic Potential for Borosilicate Glasses

M. Wang; M. M. Smedskjaer; J. C. Mauro; M. Bauchy

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA 2. Aalborg University, Denmark 3. Pennsylvania State University, USA

Molecular dynamics simulations of borosilicate glasses are notoriously challenging due to various coordination states exhibited by boron atoms, which can be 3- or 4-fold coordinated. Here, we present a new empirical force-field for modified borosilicate glasses. Although the potential retains a simple formulation (2-body interactions, fixed partial charges, constant parameters), it is found to offer an excellent transferability to a wide range of compositions, from silicate to borate glasses. The evolution of the coordination number of boron atoms upon varying glass compositions is well reproduced.