DSL2020

16th International Conference on Diffusion in Solids and Liquids
29 June – 03 July, 2020 / MALTA

Mechanistic understanding and quantitative prediction of diffusion from atomistic simulations

Erich Wimmer

Materials Design, Inc.

The deep understanding of diffusion mechanisms and quantitative predictions of temperature-dependent diffusion coefficients are now possible at an unprecedented level of detail and accuracy due to the remarkable capabilities of advanced atomistic simulations. This will be illustrated for diverse systems including diffusion processes in Li-ion batteries, fuel cells, hydrogen in steel and zirconium alloys, diffusion of defects in solids, diffusion in molten metals, molten salts and organic liquids, and oxygen diffusion related to corrosion. An overview of current theoretical and computational approaches will show their domains of validity and it will reveal opportunities for improvements and innovation, especially in the context of machine learning.