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Sintering of Alumina Nanoparticles: A Comparison of Interatomic Potentials by Atomistic Simulations

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Sintering of alumina nanoparticles is of interest both from the view of fundamental research as well as for industrial applications. Atomistic simulations are tailor-made for understanding and predicting the size-, time- and temperature-dependent sintering behavior. However, the quality and predictability of such analysis are strongly dependent on the performance of the underlying interatomic potentials. The dependence is even stronger, particularly for the oxide materials. In this work, we study the sintering of alumina nanoparticles by molecular dynamics simulations with four interatomic potentials [1, 2, 3, 4], through which we investigate the performance of the potentials.

To analyze the results, we develop a number of tailored data analysis approaches that are able to characterize and quantify the sintering process. Subsequently, the disparity in the sintering behavior predicted by the potentials is critically discussed. We also emphasize the often ignored need for multiple sintering characterizing parameters while studying sintering by molecular dynamics simulations.

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