

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Critical particle size where the Stokes-Einstein relation breaks down¹ ZHIGANG LI, Hong Kong University of Science and Technology — The validity of the Stokes-Einstein (SE) relation for particle diffusion in the nano and molecular scales has attracted much interest, but the results in the literature are controversial. In this work, it is shown that there exists a critical particle size where the SE relation breaks down by comparing particle transport in the macro- and molecular scales. Using molecular dynamics simulations, we study the critical size and find that the van der Waals force plays an important role in particle diffusion as the particle size approaches molecular scale. Due to the limitations of computing facilities, we could not find exactly where the critical particle size is, but the simulation results qualitatively predict that this critical size is of a few nanometers.

¹This work is supported by the Hong Kong Innovation and Technology Fund under Grant No. GHP/035/07GD

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Date submitted: 19 Nov 2009

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