UNIVERSITÄT DUISBURG ESSEN

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Charged Particles' Transport in Conductive Porous Media: A Molecular Dynamics Study

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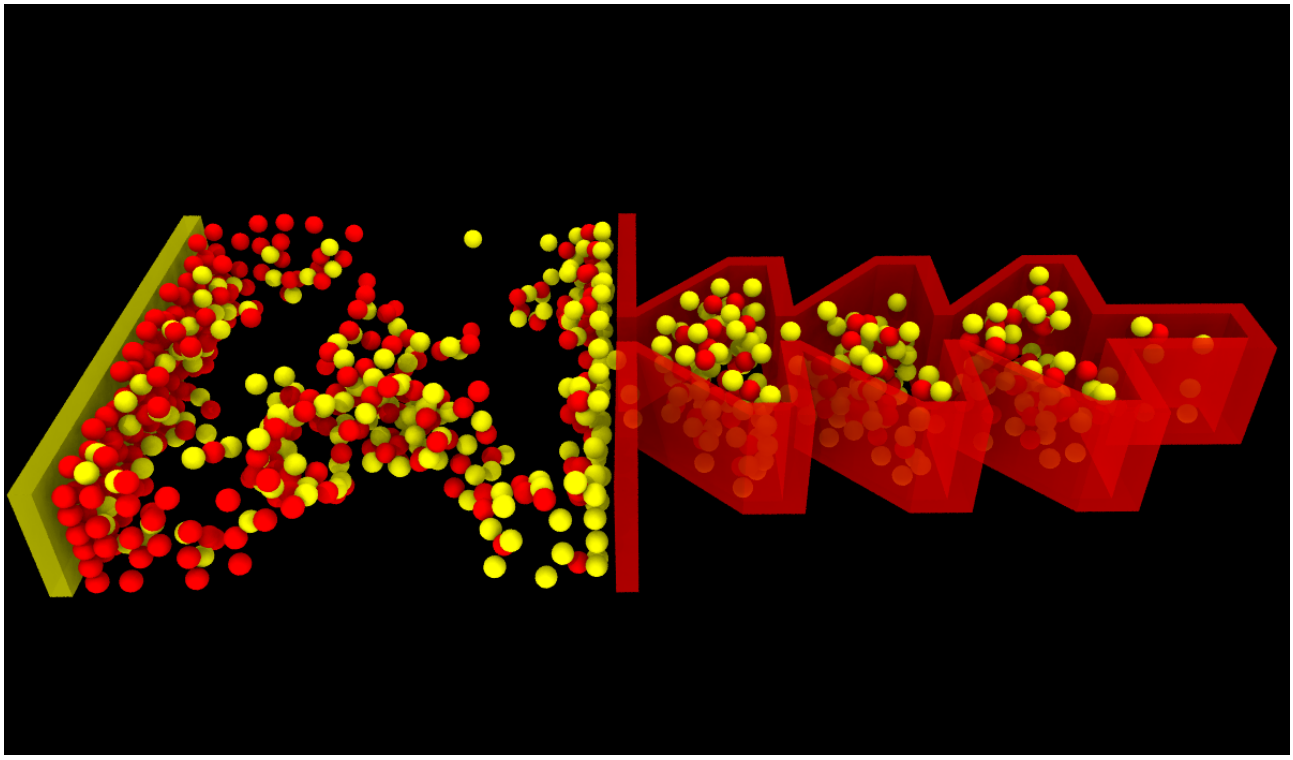

Transport of charged particles in a conductive porous media is a well-known phenomena for scientists and engineers. It has numerous applications from electrical power storage devices such as supercapacitors and batteries, to novel techniques of water desalination. Because of the complexity of theoretical and experimental studying of these systems, numerical simulation is a main tool to investigates them. However, the existence of long-range electrical interaction between charged particles themselves as well as charged particles - walls' conductive pore, ordinary molecular dynamics methods fails to simulate such systems.

There are a few methods to model such complex systems, one of them is called the Poisson to Laplace Transform (PLT) algorithm. In this talk, we will start from a general review of physics and applications of transport of charged particles in conductive porous media, then a brief review of the PLT algorithm and its implementation in the CAVIAR package will be presented.

At the end, we will discuss the results of some MD simulations of different systems.