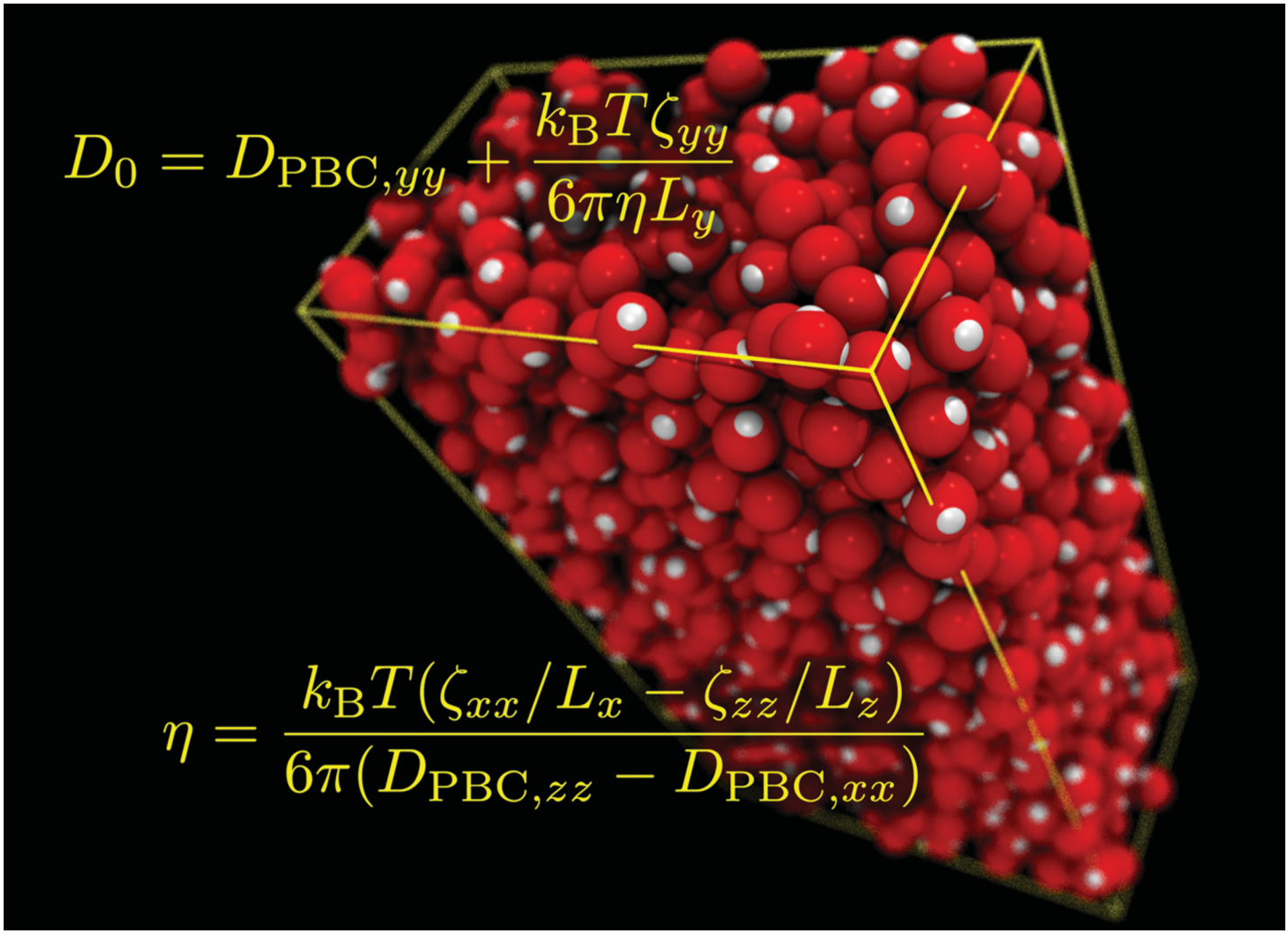

Showcasing research from Johanna Busch and Dietmar Paschek from the Institute of Chemistry at the University of Rostock, Germany.

An OrthoBoXY-method for various alternative box geometries

This work extends on a new and efficient way to compute viscosities and true system size independent self-diffusion coefficients from Molecular Dynamics simulations. By exploiting the effect of hydrodynamic interactions between particles in systems with periodic boundary conditions, simple exact formulae are derived that allow the computation of those properties based on direction-dependent self-diffusion data obtained from periodic systems with orthorhombic unit cells of arbitrary shape.

As featured in:

See Johanna Busch and Dietmar Paschek, *Phys. Chem. Chem. Phys.*, 2024, **26**, 2907.

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