

Determining the shear viscosity of a solvent in the presence of electric fields

Zoran Miličević^{1,2}, David M. Smith^{3,4}, Ana-Sunčana Smith^{1,2}

¹*Institut für Theoretische Physik, Universität Erlangen-Nürnberg,
Staudtstraße 7, 91058 Erlangen, GERMANY*

²*Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg, Nägelsbachstraße 49b, 91052 Erlangen, GERMANY*

³*Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, CROATIA*

⁴*Computer-Chemie-Centrum, Universität Erlangen-Nürnberg,
Nägelsbachstraße 25, 91052 Erlangen, GERMANY*

The shear viscosity is a very important kinetic property characterizing the macroscopic properties of molecular systems and is hence useful for the parametrization of reliable force fields. However, calculating the shear and bulk viscosities from molecular dynamics simulations is still a challenging task.

Here we study the shear viscosity of water by performing extensive MD simulations using the GROMACS software package and different models of water (e.g., SPC/E and TIP4P) as a function of the electric field strength. The latter breaks the otherwise isotropic nature of the solvent. The shear viscosity is related to the autocorrelation function of the off-diagonal elements of the pressure tensor by the Green-Kubo relation, which is used to analyze pure water simulations. Alternatively, the viscosity is calculated from the mobility of a spherical particle, the latter arising from the diffusion constant evaluated in independent simulations. Apart from the fact that different treatments show excellent agreement, we find that the field decreases the component of the shear viscosity perpendicular to the field and increases the components parallel to the field.