CONFERENCE ABSTRACTS

International Student Conference

“Science and Progress”

DAAD

Санкт-Петербургский государственный университет

Freie Universität Berlin

German-Russian Interdisciplinary Science Center

St. Petersburg — Peterhof
November, 9–11
2021

CONFERENCE ABSTRACTS
International Student Conference “Science and Progress” —
SPb.: SBORKA, 2021-224 p.p.
ISBN 978-5-85263-109-1

Calculation of the Viscosities of Polar and Nonpolar Solutions by Molecular Dynamics Method

Polovinkin Mikhail, Volkov N.A., Adzhemyan L.Ts., Shchekin A.K.

polovms@gmail.com

Saint Petersburg State University, Saint Petersburg, Russia

Calculation of viscosities of colloidal systems via molecular dynamics simulations can be done, e.g., with the help of the Stokes-Einstein formula [1, 2]. In this paper we use the method proposed by Palmer in [3] and implemented in GROMACS 2020 software package for estimating the viscosities of one- and two- component molecular liquids. This method is based on computation of the autocorrelation functions of the momentum. It has been here applied for finding the viscosities of several homogeneous molecular systems (water, pentane, heptane, decane) and that of a weakly inhomogeneous system, i.e., a small premicellar aggregate of non-ionic surfactant molecules (C12E4) in heptane. In particular, the viscosity was calculated for systems containing monomer, dimer, and tetramer of C12E4 molecules. All the systems were represented by the all-atom models within the CGenFF 4.4 force field [4] and were simulated via molecular dynamics in the NPT statistical ensemble. Good agreement of our results for the one-component liquids with the previous works was observed. For the systems containing SPC and SPC/E water molecules, the results are consistent with those in [5]. The results for the viscosity of pentane coincided well with the computer simulation results in [6]. For the system consisting of decane molecules, the general agreement of our simulation data on viscosity with the experimental data [7] was observed. We plan to use this method for calculating the viscosities of the systems containing bigger aggregates (reverse micelles).

Acknowledgments: This work was supported by a grant RFBR 20-03-00641_A from the Russian Foundation for Basic Research.

References

1. Volkov N.A., Shchekin A.K., Tuzov N.V., Lebedeva T.S., Kazantseva M.A. *J. Mol. Liq.*, **2017**, *236*, 414-421.
2. Volkov N.A., Eroshkin Yu.A., Shchekin A.K., Koltsov I.N., Tretyakov N.Yu., Turnaeva E.A., Volkova S.S., Groman A.A. *Colloid J.*, **2021**, *83*, No 4, 406-417.
3. Palmer B.J. *Phys. Rev. E*, **1994**, *49*, 359-366.
4. Vanommeslaeghe K., Hatcher E., Acharya C., Kundu S., Zhong S., Shim J., Darian E., Guvench O., Lopes P., Vorobyov I., Mackerell Jr. A.D. *J. Comput. Chem.*, **2010**, *31*, 671-690.
5. Hess B. *J. Chem. Phys.*, **2002**, *116*, 209-217.
6. Kondratyuk N.D., Orekhov M.A. *J. Phys. Conf. Ser.*, **2020**, *1556*, 012048.
7. Naake L.-D., Wiegand G., and Franck E.U. *Z. Phys. Chem.*, **2002**, 216, 1295-1310.