We have developed a molecular theory based on mode coupling approach where ultrafast solvation in 3PEPS measurements has been explained in terms of solute-ionic liquid non-dipolar interactions [J. Chem. Phys. 2012, 137, 114501]. Relation between single particle rotation and Stokes shift dynamics has been explored (see Figure1). Our analyses suggest different experimental techniques probe different components of the total solvation energy relaxation of a laser-excited dye in a given ionic liquid.

Our all-atom molecular dynamics (MD) simulations on ionic liquid (IL), 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF$_6$]), have revealed that the ratio between the simulated reorientation time constants, $\langle \tau_1 \rangle / \langle \tau_2 \rangle$, differs considerably from 3 at 450 K, indicating presence of significant heterogeneity effects even at this high temperature [Theo. Chem. Acc. 2013, 132, 1348].

Our all-atom MD simulations on aqueous reverse micelles have revealed that nanosecond confined aqueous dynamics reported by fluorescence measurements is indeed real and originates from slow water [J. Phys. Chem. B 2013, 117, 3345].

Our fluorescence measurements with polymer-electrolyte composite, [0.85 PEG + 0.15\{f KNO$_3$ + (1-f) LiNO$_3$\}], have revealed presence of spatio-temporal heterogeneity which disappears in the absence of any electrolyte or at higher temperatures [J. Chem. Phys. 2013, 138, 114909].
PUBLICATIONS IN JOURNALS


9. Sanchayita Rajkhowa, Anuradha Das, Sekh Mahiuddin and Ranjit Biswas, *Specific Conductivities and Viscosities of 0.1LiNO3 + 0.9 [xCH3CONH2 + (1 – x)CO(NH2)2] as Functions of Mole Fraction, x, and Temperature*, Journal of Chemical Engineering Data, 2012, 57, 3467-3472.


BOOKS PUBLISHED


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