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Hydrogen-bonding and dielectric response of N,N-dimethylacetamide aqueous solutions under E/M fields using molecular dynamics

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ABSTRACT

Non-equilibrium molecular dynamics (NMD) simulations of the N,N-dimethylacetamide (DMAC) aqueous solutions using a non-polarizable field have been performed in the frequency of 1 GHz with the intensity of the E/M field in the range of 0 to 3×10^9 V/m. The principal term in the radial distribution function reveals significant differences in the structure and reorientation dynamics of DMAC–H_2O interaction, indicating a substantial field-induced effect of molecular structure on the hydrogen-bond network. The first hydration shell alters significantly with increasing E/M field strength. When the intensity of the E/M field is above 3×10^8 V/m a threshold effect is observed, and the static dielectric constants decrease with increasing E/M field strength. And the molecular polarizability gradually increases when the E/M field strength increases. The average hydrogen-bond number and hydrogen-bond lifetime decline with the E/M field strength.

1. Introduction

Microwave energy has been directly applied in many fields but there are difficulties such as the transfer of laboratory experiment system to industrial applications. The successful application of microwaves is directly associated with the dielectric properties of the materials. An accurate estimation of dielectric properties of materials is beneficial for microwave application in chemical reaction, microwave-assisted chemistry and other fields [1].

As a strong polar aprotic solvent, DMAC is widely used in synthetic materials, petroleum chemical, reaction catalyst, electrolytic solvent, adhesive industry, as well as a variety of crystalline adduct and complex [2] due to the unique physical and chemical properties [3–5]. The interest in DMAC also own to it is more stable, presumably due to hydrogen-bond or dipole–dipole interactions between the external N – H bond and the solvent [6]. The synthesis of Ag nanoparticles can be quickly completed [7] within DMAC solutions. In an effort to cast light on DMAC's action, the DMAC–water system has been studied by using a variety of experimental and theoretical techniques, such as, X-ray [8], NMR [9], infrared [8], gas electron diffration [10] and dielectric spectroscopy [11–13], all of which shed light on a different aspect of the interaction of DMAC with water.

Although N.J. English and Sanghun Lee et al. have shown that polarizable force fields such as AMOEBA, TIP4P-FQ, and CHARMMA can provide accurate information on polarization effects [14–20]. Molecular dynamic with electronic continuum (MDEC) model obtained a dielectric constant of carbonate molecules using non-polarizable fields, whose values are satisfied with the experimental data [21,22]. In addition our applied external electric field almost exceeds the strength of experimental or industrial realizable field, which indicates that hydrogen bonds and weak inter molecules interactions are similar in solutions using a polarizable field. But conversely hydrogen bonded effects are distinguished feasibly using a non-polarizable field. So we believe that the dielectric properties of DMAC aqueous solution using non-polarizable force fields provide a chance for testing a potential MDEC model's predictive capabilities under an electric field in GROMACS package.

Therefore, in this paper dynamics and structures of DMAC aqueous solutions non-polarizable fields such as RDF, coordination number, static dielectric constant and average hydrogen-bond number under E/M field are performed using a non-polarizable force field.

2. Computational method

2.1. Interaction potentials and simulation details

The simulations were performed using a modified version of the GROMACS 4.5.5 [23] simulation package with the TIP4P [24] model and the OPLS-AA potential characterizing the water and DMAC molecules, respectively. The simulations involved 555 water molecules placed in a cubic simulation periodic box and two concentrations, i.e. 0.8 M and 8 M (molality), corresponding to 8 DMAC molecules and 80 DMAC molecules respectively. TIP4P water molecules were added to the system from a relaxed liquid configuration at 298 K and 1 bar.

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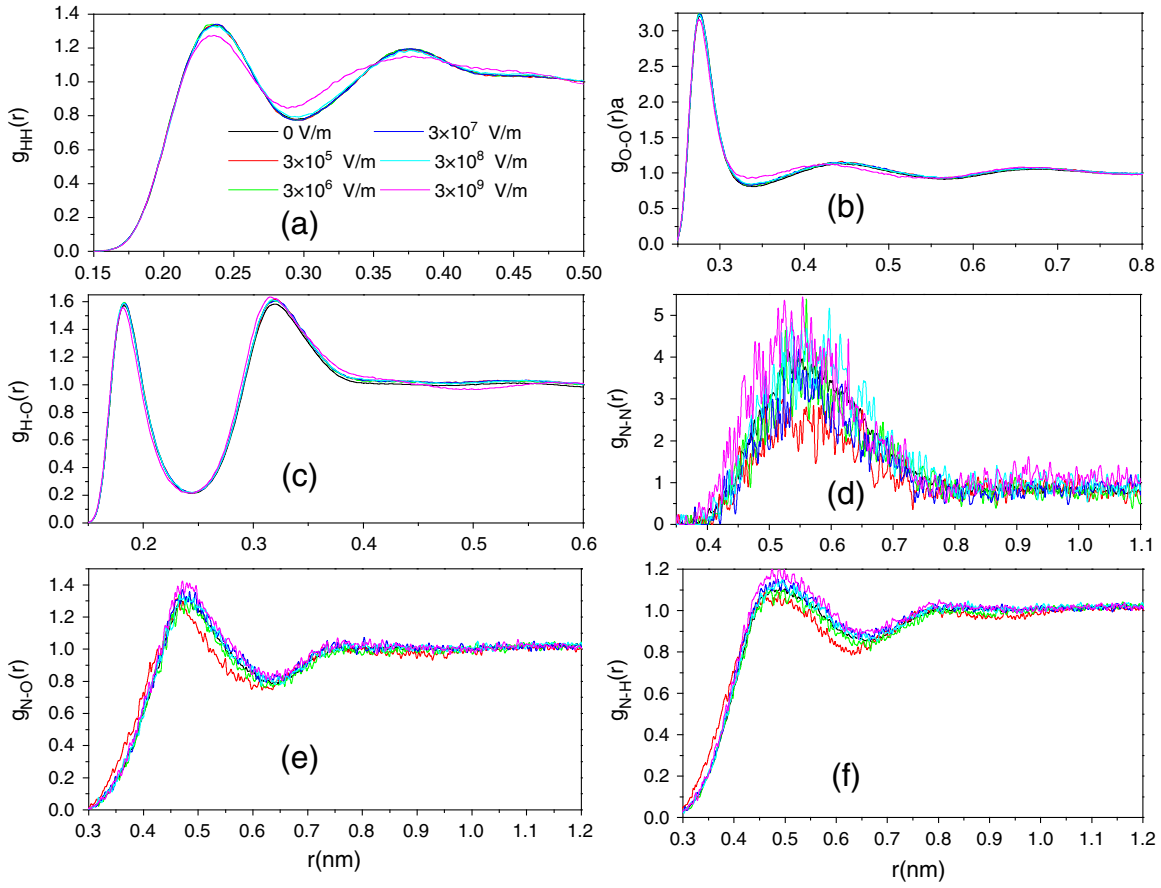

Fig. 1. RDF of 0.8 M DMAC aqueous solution with and without applied E/M field. (a) H – H, (b) O – O, (c) H – O, (d) N – N, (e) N – O and (f) N – H.

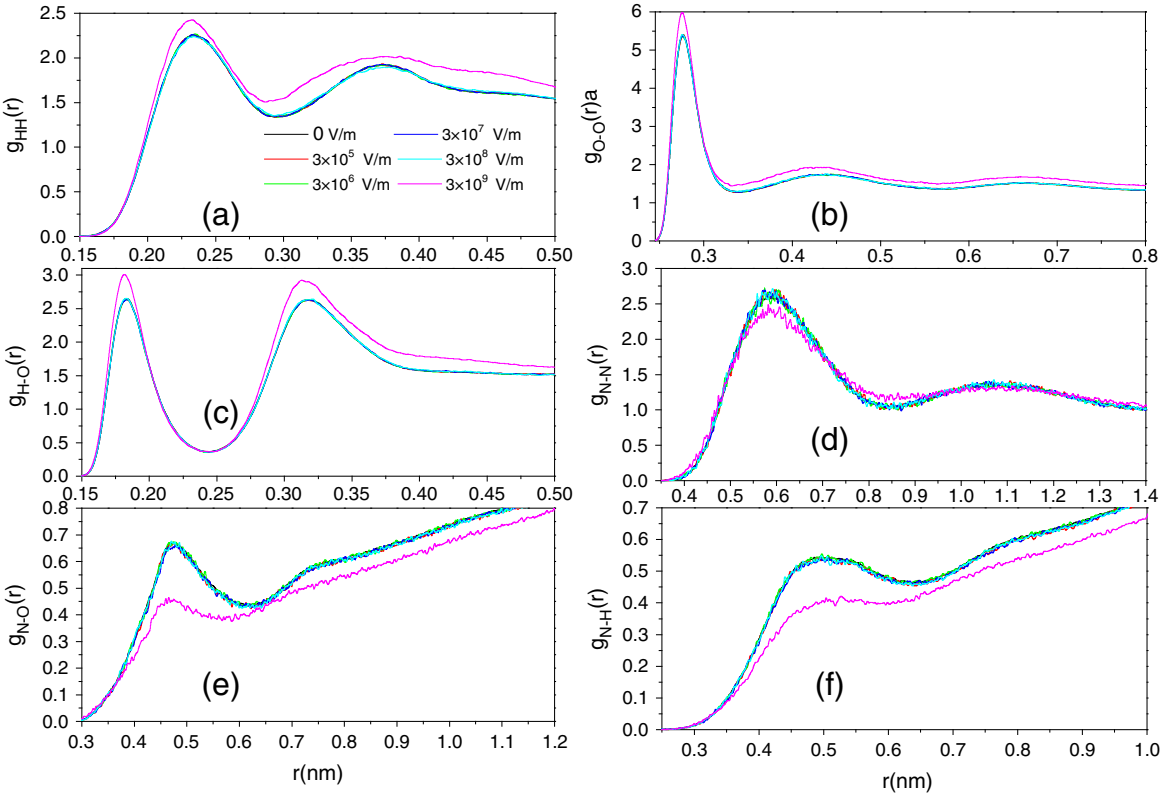

Fig. 2. Radial distribution functions of 8 M DMAC aqueous solution with and without applied E/M field. (a) H – H,(b) O – O, (c) H – O, (d) N – N, (e) N – O and (f) N – H.