Screened potential constraint in a Reverse Monte Carlo (RMC) simulation

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Résumé : (16 gras)

Introducing a potential as additional constraint in the RMC modeling, one could obtain some better results. Mismatch between the interaction potential between charges of atomic or molecular species in the system would be taken into account and the method of RMC simulation based on experimental data. Consequently, we could suggest that the choice of the interaction model as a function of atomic or molecular properties forming the system could bring a meaningful improvement to the results.

Abstract :

RMC is generally limited to explore structural property of a system with or without interaction model. Some artifacts have appeared in structural modeling results. To remedy this, a potential model is introduced to the modeling calculation RMC. *Introducing the proposed potential as constraint, an improvement in the coordination of the structural function is noticed.*

Key words: ***RMC Modeling, Aqueous Electrolyte, Screened Potential***

1 Introduction

To explore a certain number of structural features of an aqueous electrolyte LiCl-6H_2O type, a Reverse Monte Carlo (RMC) modeling is applied [1, 2] .

2 Paragraph

This is based essentially on neutron scattering data [3, 4] consisting of four partial distribution functions issue from the technique of the isotopic substitution. Instead of introducing the interaction potential as in the classical methods (MD, MC), one computes a parameter χ^2 representing the difference between the calculated structure function and that are of the experiment within standard deviation. It is expressed as:

$$\chi^2 = \sum_i \left[G^{RMC}(r_i) - G^{EXP}(r_i)\right]^2 / \sigma^2(r_i)$$

One examines the system at glassy (120K) and liquid (300K) state compared to pure water at room temperature. The chlorine and lithium ions charged -1 and +1, respectively, the water molecule is represented by a flexible model [8] charged as -0.8476 for the oxygen and +0.4238 for each hydrogen atom [7, 8]. The results one obtains could include some artifacts [5, 6]. To remedy for this, we could make a propose choice of screened potential model.

$$u_{ij} = k\frac{\alpha_i e^2 \exp(-\kappa r)}{r}$$

α_i charge fraction species i, $r = r_{ij}$ distance between two different species, k coulomb potential parameter and κ is the screen constant respectively. Thus statistical parameter χ^2 becomes:

$$\chi^2 + wU/k_BT$$

where w represents a weight to be unit in our case.

Introducing potential as constraint in RMC simulation suggests a useful test of an interaction potential model for classical methods as Monte Carlo (MC) and Molecular Dynamic (MD) with which one can compute thermodynamic properties

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