Computer Simulation of 1,2-dichloroethane Liquid Under External Electric Field

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Abstract

Molecular dynamics simulation was carried out for liquid 1,2-dichloroethane under an external electric field. Various types of electric fields including the direct current field, the alternating current field and the positive-half-period cosine field were applied on the system. The maximum applied field strength is $100 \times 10^4 \text{V/m}$ and the maximum frequency of alternative current and positive-half-period field is $10^{12}$ hertz. Results of simulation showed that the form and strength of external field affects the populations of trans and gauche configuration in different ways. Under a strong direct current field it was found that all trans configurations are converted completely into gauche configurations. Order parameter and the correlation function of the torsion angle of the system depended on both the form and the strength of applied field. The maximum value of the order parameter was found to be 0.56 under a strong direct current field.
shows obviously that $P_{\text{trans}}$ is decreasing and $F_{\text{gauche}}$ are increasing along with the field strength. When the external field strength is over $75 \times 10^6 V/m$ all trans configuration is converted into gauche configurations. Given in Figure 2(b) are the $P(\phi)$'s of the systems under external AC fields with same frequency ($\omega = 10^{12}$ hertz) but different field strengths. $P(\phi)$'s of the systems without external field and under DC ($E = 50 \times 10^3 V/m$) are also shown in this figure for comparison. The figure shows that $P_{\text{trans}}$ is decreasing very slowly (compared to the DC field) with increasing of the field strength. Given in Figure 2(c) are $P(\phi)$'s of the systems under PHPC fields. $P(\phi)$'s of systems of no field, and under a particular DC and an AC field are also shown for comparison. The figure shows that when the strength of the PHPC field is less than $25 \times 10^4 V/m$, $P_{\text{trans}}$ is larger than the system without external field or larger than the system under AC field with same strength. On the other hand, when the strength of the PHPC field is over $50 \times 10^4 V/m$, $P_{\text{trans}}$ is less than the system without external field. $P_{\text{trans}}$ and $P_{\text{gauche}}$'s of the system under PHPC field are found very close to the system under DC field with half of the field strength. In summary, $P_{\text{trans}}$ and $P_{\text{gauche}}$'s of the system are sensitive to the form and strength of applied field. According to our simulation, it is possible to eliminate trans configuration completely by using AC field.

In summary, by means of molecular dynamics simulation the liquid 1,2-dichloroethane system under various external electric fields was investigated. The simulation shows that the populations of trans and gauche configurations can be either increasing or decreasing when the system is interacting with different external fields. The significance of this result is that it may be possible to control the population of specific configurations of 1,2-dichloroethane liquid by properly selecting the form and strength of external field. From our simulation we found that strong DC field causes the conversion of trans configuration into gauche configuration completely. External AC field can also have similar effect but with much smaller conversion extent than DC field. Weak PHPC field causes the increasing of trans configuration but strong PHPC field causes the increasing of gauche configurations. The investigation of the order parameter of the systems shows that the dipole moment of 1,2-dichloroethane molecule tends to align along the direction of the external DC and PHPC fields. The larger the strength of DC
Fig. 2 Population of torsion angles of systems under DC, AC and PHC fields.