



Investigation of binding energy of heavy gases with a polymeric surface using molecular dynamics simulation

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Abstract

One method of checking the stability of a molecular dynamic (MD) simulations is the Binding energy (E_{binding}) of the system over time. Binding energy (E_{binding}) between two components, can reflect how well the two components mix with each other, which is defined as the negative of the intermolecular interaction energy (E_{inter}). In this paper, using the MD method, the polymer surface of DGEBA and TETA hardener is simulated and then the binding energy is determined to evaluate the stability of the system. The amount of binding energy related to the interaction of heavy gases of uranium hexafluoride, tellurium hexafluoride and sulfur hexafluoride with the polymer surface is determined at different times and temperatures. For interaction of uranium, tellurium and sulfur hexafluoride gas molecules with polymeric surface, the binding energy increases to -100, -110 and -130 Kcal/mol, respectively.

Keywords: Binding energy, polymer surface, uranium hexafluoride, tellurium hexafluoride

Introduction

The binding energy is a measure of the energy of interaction between two components. Together with the coordination numbers, it enables generation of the mixing energy and the chi parameter and of phase diagrams [1]. In evaluating binding energies, it is important to take into account and to properly weight a large number of relative orientations of the two molecules. Blends generates a large number of molecular orientations and calculates the pair interaction energies of each configuration. By employing a sampling technique that includes excluded-volume constraints, Blends is able to sample from predominantly energetically favorable configurations. The excluded-volume constraint method is a modified version of the molecular Silverware algorithm (Blanco, 1991), which combines molecules so that their van der Waals surfaces are in contact [2]. Non-bonded interactions include short-range and long-range interactions. Electrostatic interactions are treated in molecular mechanics by pairwise calculation using the Coulomb law. Electrostatic interactions play an essential role in biological and technological processes. From ion motion in batteries to protein function in living cells, charge modulation dictates the function of processes that involve ions[3].

Due to the importance of stability in molecular dynamics simulations, in this paper the stability of the interaction of heavy gases with the polymer surface was investigated using binding energy calculations.

Methodology

The Blends Binding energies task allows you to efficiently sample the energy of interaction between specified molecules [4]. This distribution is sampled by generating a large number of pair configurations in which the van der Waals surface of the two molecules are in contact. The binding energy (E_{binding}), which is defined as the negative value of the interaction energy (E_{inter}), is a measure of the compatibility between two components mixed with each other [5]. A negative E_{binding} represents poor compatibility between two components. On the contrary, a positive E_{binding} represents good compatibility, and a larger positive value indicates better compatibility. From the equilibrium system at the systems and the individual components can be evaluated. The intermolecular interaction energy can be extracted by the total energy of the mixture and total energies of each component in the equilibrium state. Thus, the binding energy between SF_6 , TeF_6 and UF_6 molecules and DGABA-TETA polymer can be determined as follows:

$$E_{\text{binding}} = -E_{\text{inter}} = E_{\text{total}} - (E_{\text{gas}} + E_{\text{Polymer}})$$

where E_{total} is the total energy of the SF_6 , TeF_6 , UF_6 /Polymer mixture, and E_{gas} and E_{Polymer} are the total energies of gas molecules and polymer surface, respectively. The studied surface is a polymer surface with a molecular structure of diglycidyl ether of bisphenol-A (DGEBA) epoxy and Triethylenetetramine (TETA) hardener. The chemical formulas of DGEBA

and TETA are $C_{39}O_7H_{44}$ and $C_6N_4H_{18}$ and their molecular masses are 624 gr/mol and 146 gr/mol, respectively. The composition ratio for DGEBA to TETA is 6/2 [6]. The molecular structure of DGEBA and TETA monomers are represented in Fig.1.

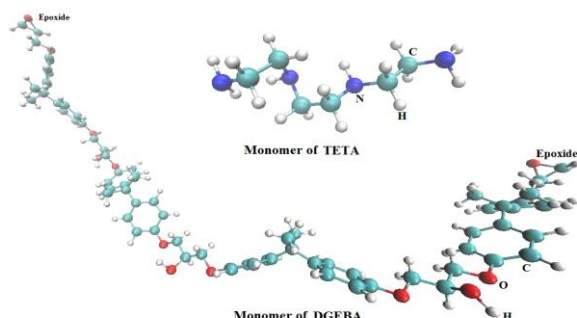


Fig.1. Molecular structure of DGEBA and TETA monomers

Results and discussion

Fig.2 shows the variation of binding energy versus time steps for interaction of the uranium, tellurium and sulfur hexafluoride molecules with the polymer surface at the temperature of 300 K during 100 ps in the MD simulation obtained from Materials Studio 2017. For all the interactions, the interaction of the gas molecules with polymer surface gradually increases. In this temperature, for uranium, tellurium and sulfur hexafluoride gas molecules, the attractive interaction with polymer surface increases to -100, -110 and -130 Kcal/mol, respectively. Negative binding energy values indicate that the interaction between gas molecules and polymer surface is favourable towards lower energy and the mixture is thus stable. As shown in the figure, as the molecular mass of the gas increases, the intermolecular and intramolecular interaction increases to -130 kcal/mol.

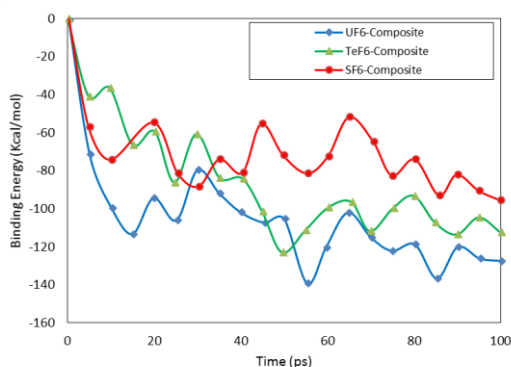


Fig.2. The binding energy evolution for interaction of SF_6 , TeF_6 and UF_6 molecules with the polymer surface during 100 ps of simulation.

Fig.3 shows the polymer temperature dependence of the binding energy. It was shown that with increasing

temperature, the interaction of uranium, tellurium and sulfur hexafluoride gas molecules with polymer surface decreases weakly and as a result the influence of temperature is neglectable.

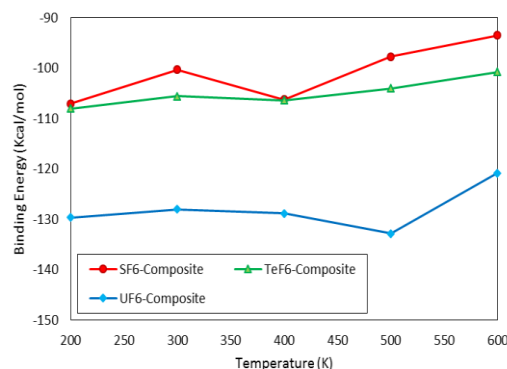


Fig.3. The variations binding energy versus temperature of polymer surface from 200 to 600 K.

Conclusions

In the molecular dynamics simulations of heavy gases with polymer surfaces it was shown that at the $T=300K$, for interaction of uranium, tellurium and sulfur hexafluoride gas molecules with polymeric surface, the binding energy increases to -100, -110 and -130 Kcal/mol, respectively and with increasing temperature, the interaction of these gas molecules with polymer surface decreases weakly.

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