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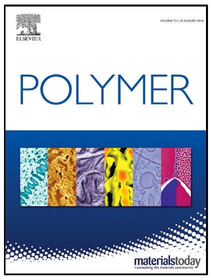

Thermodynamic analyses of the hydrogen bond dissociation reaction and their effects on damping and compatibility capacities of polar small molecule/nitrile-butadiene rubber systems: molecular simulation and experimental study

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Thermodynamic analyses of the hydrogen bond dissociation reaction and their effects on damping and compatibility capacities of polar small molecule/nitrile-butadiene rubber systems: molecular simulation and experimental study

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Although the hydrogen-bonding damping theory of polar small molecule/polymer systems is widely accepted, optimal selection of small molecules and the ration of that with polymer is rarely achievable. Herein, we report a new molecular simulation way to attempt solving the above problems. A key point is to introduce the thermodynamic analyses of hydrogen bond dissociation reaction (HBDR). According to hydrogen-bonding damping theory, under the premise that Gibbs free energy is negative, the higher enthalpy, lower reaction equilibrium constant (K^{Θ}), plus higher derivative of lnK^{Θ} to temperature of HBDR will lead to a better damping capacity. The above parameters obtained through quantum mechanics indicated that the relative damping capacity of three systems is AO-80/NBR > AO-70/NBR > AO-60/NBR. Unified linear relationship (R^2 = 0.924) between normalized parameters (damping parameter (tan δ_{max}) and energy dissipation parameter calculated by the thermodynamic parameters) was discovered in the combined three homogeneous systems. This work may help us better understand the structure-property of polar small molecule/polymer systems, and further provides new insights into the screening and design of high damping materials.

Keywords: thermodynamic analyses, hydrogen bond dissociation reaction, damping properties, molecular simulations, linear regression analyses