Journal of Material Sciences & Engineering

Lennard-Jones potential and the enthalpy of formation of a binary solution

Alexander Levinsky

University of Applied Sciences, Germany

Abstract

A semi-empirical formula is derived that describes the dependence of the enthalpy of formation of a binary solution on its composition x (mole fraction of the first component in the solution):

$$n_1 = \frac{x\rho}{\mu_1 x + \mu_2(1-x)}; \quad n_2 = \frac{(1-x)\rho}{\mu_1 x + \mu_2(1-x)}; \quad n = n_1 + n_2;$$

$$\Delta H = A_{11}(n_1^2 - xn_{10}^2) - B_{11}(n_1^2 n^2 - xn_{10}^4) + A_{22}[n_2^2 - (1-x)n_{20}^2] -$$
$$-B_{22}[n_2^2 n^2 - (1-x)n_{20}^4] + 2A_{12}n_1 n_2 - 2B_{12}n_1 n_2 n^2$$

With ρ – the density of the solution;
μ_1 and μ_2 – the molar masses of the components;
n_1,n_(2) and n – the numbers of moles of the components per unit volume of the solution;
n_10 and n_20 – the numbers of moles per unit volume of pure components;
A_ij – the „trimming" parameters associated with Lennard-Jones potential parameters.
The formula is in a good agreement with experimental data.

Biography

Alexander Levinsky worked as University chemical faculty. Scientific assistant at Institute for Polymer Research, Self-organization in the mass-polymerizing methyl methacrylate, Thermodynamics of the solutions, Viscosity of the concentrated suspensions, Instrument-based analytics, Development of the measuring systems. He also worked as Head of research and development department at Bekro Chemistry ltd Colorimetry, coloristics. Freelance lecturer at University of Applied Sciences Lectures in mathematics, physics and chemistry. Currently he is retired.

5th International Conference on Physical and Theoretical Chemistry
December 06, 2021

Citation: Alexander Levinsky, Lennard-Jones potential and the enthalpy of formation of a binary solution, 5th International Conference on Physical and Theoretical Chemistry, December 06, 2021, 05