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Y. Kalyuzhnyi, A. Jamnik

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# Shielded attractive shell model of polymerizing hard spheres of different size. Resummed thermodynamic perturbation theory and computer simulation

Y. Kalyuzhnyi<sup>a,\*</sup>, A. Jamnik<sup>b</sup>

<sup>a</sup>*Institute for Condensed Matter Physics NASU, Lviv, Ukraine*

<sup>b</sup>*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia*

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## Abstract

Resummed thermodynamic perturbation theory for central force associating potential is extended and applied to study the properties of shielded attractive shell model of polymerizing hard spheres of different sizes. The model is represented by the two-component mixture of hard spheres with additional square-well interaction treated in the sticky limit and located inside the hard-core region and acting only between particles of different species. The theory self-consistently takes into account the changes in the excluded volume of the system due to bonding of the particles. Theoretical predictions for the pressure and fraction of the particles in different bonding states at different temperatures and densities are compared against computer simulation predictions. The theory appears to be very accurate in description of the dimerizing and trimerizing versions of the model. For the model, which allows chain polymerization the theory is slightly less accurate, in particular for low temperatures and high densities.

### *Keywords:*

Thermodynamic perturbation theory, association, sticky potential, polymerization.

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\*Corresponding author

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