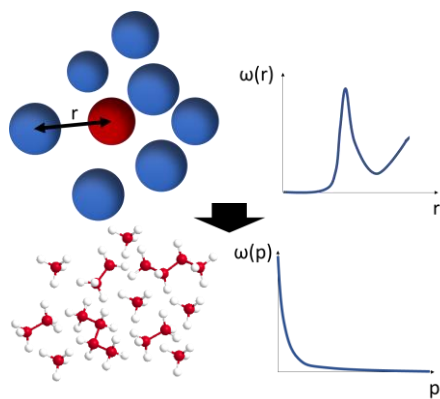


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|--|---|
| <input checked="" type="checkbox"/> Bachelor Thesis | <input checked="" type="checkbox"/> theoretical |
| <input checked="" type="checkbox"/> Plant Design Practice (KÜ) | <input type="checkbox"/> experimental |
| <input type="checkbox"/> Master Thesis | <input type="checkbox"/> constructive |

Topic: Deriving the associate distribution from a radial distribution



A novel model is developed to describe associating isomers. It describes the association of molecules via chemical theory. Chemical theory considered association as a chemical reaction with an assigned equilibrium constant. The formed clusters, called associates, can be described with a distribution. This distribution is then further used to describe the thermodynamic properties of the mixtures.

To validate the distribution, it should be compared with results from literature. Molecular dynamic simulations as well as experimental investigations often give the resulting distribution of particles in a radial distribution function.

Within the scope of this work, a new method is to be developed for converting possible radial distributions into a distribution of associates.

Contact: Dipl.-Ing. Gottfried Segner
segner@tugraz.at
+43 (316) 873 – 7460

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