MSc graduation project

Phase Equilibrium and Interfacial Free Energy Determination of Sugar Alcohols with Molecular Modeling

Introduction

Heat storage systems are widely used in different applications. Phase Change Materials (PCMs) have long been proposed as one important category of heat storage media. Recent advancement in PCM development ascribes to the discovery of a promising class of materials – Molecular Alloy based Sugar Alcohols (MASAs). These materials have large melting enthalpy, moderate melting temperature and significant subcooling effects, and therefore are very promising in seasonal storage applications. However the slow kinetics in the nucleation and crystal growth process remain to be improved. This task relies on a more detailed understanding of the thermodynamics and kinetics on molecular level. We apply first principle molecular modeling method to numerically predict the phase equilibrium and anisotropic interfacial free energies of selected sugar alcohols of interest. These properties control the morphology and kinetics in crystal growth and hence are key design parameters in new MASA developments. The project is under the EU project 'SAM.SSA' framework in collaboration with Fraunhofer, CNRS, and 6 other research institutes or companies.

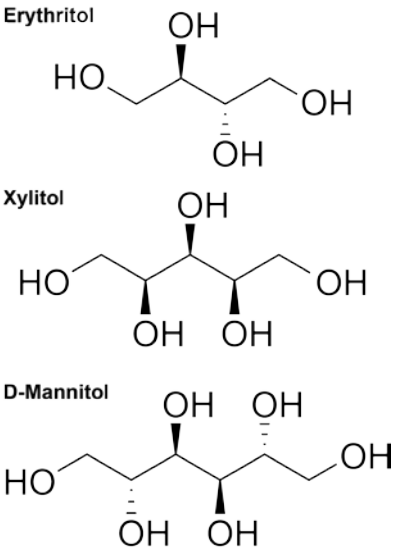

Figure 1. Example of sugar alcohols

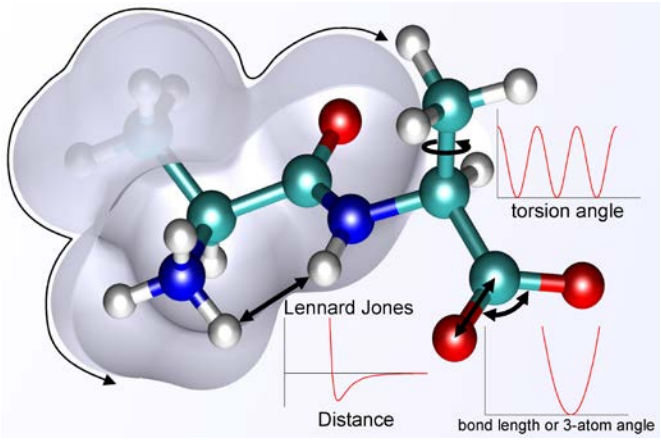

Figure 2. Molecular modeling

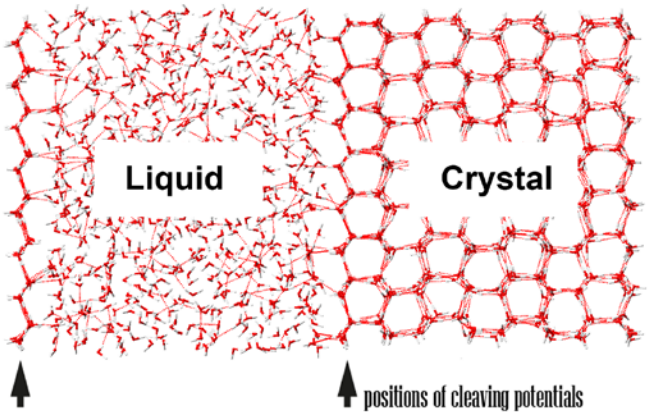

Figure 3. Water simulation with cleaving potential

Methodology

Classical application of molecular dynamics (MD) is to determine equilibrium properties from ensembles. Here, we steer the molecules with artificial external potentials to achieve a more efficient Boltzmann sampling.

Tasks

- Master the background knowledge of free energy calculation methods and molecular simulations
- Design efficient external cleaving potentials
- Calculate anisotropic interfacial free energies
- **Publish an academic paper** (adviced)

Requirements

- Keen to solve and contribute to global energy problems
- Good analytical and communications skills
- Basic knowledge of molecular modeling and statistical physics

We Offer

- A challenging task at a dynamic and ambitious university and in an enthusiastic team
- A good entry towards state of art theoretical research and a good opportunity to **publish papers**
- A consortium of 9 research institutes/companies from Germany, Spain, UK, France and Netherlands

Please feel free to contact:
Ir. Huaichen Zhang, h.zhang@tue.nl, GEM-Z 2.118
Dr. Silvia V. Nedea, s.v.nedea@tue.nl, GEM-Z 2.122

SAM SSA