Combining COSMO-RS with other models leading to improved property predictions

Sebastian Kaminski, Kai Leonhard
Chair of Technical Thermodynamics, RWTH Aachen University, Germany

**Motivation**
- Avoid experimental effort for obtaining property data
- Predictive models not yet accurate enough for certain tasks

50 non-polar components: linear & branched alkanes, alkenes, esters, ethers, ketones, aldehydes, cyclics. Average over broad temperature range is shown. On average, all predicted properties improve.

**Idea**
Combine information from independent predictive models to increase accuracy of property predictions

---

**Further Information**
Sebastian Kaminski
RWTH Aachen University
Chair of Technical Thermodynamics
Schinkelstr. 6, 52056 Aachen, Germany
E-Mail: sebastian.kaminski@lt.rwth-aachen.de
Phone: +49 241 80 95 918

**Acknowledgements**
This work was performed as a part of the Cluster of Excellence TaiMak Fukl from Bionic funded by the Excellence Initiative by the German federal and state governments to promote science and research at German universities.

---

**References**

---

**PCP-SAFT equation of state**

- Combination with log-likelihood equation

- Parameters of the original predictive PCP-SAFT model have been refined
- A total of 13 adjustable model parameters (not substance-specific) are used