Martin Thomas Horsch, Simon Stephan,
Hans Hasse, and Jadran Vrabec

Science & Technology Facilities Council | UK Research and Innovation

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN | LEHRSTUHL FÜR THERMODYNAMIK

berlin

Molecular model database of the Boltzmann-Zuse Society for Computational Molecular Engineering

Computational Molecular Engineering

VIMMP
VIRTUAL MATERIALS MARKETPLACE

15th October 2019

DACOMSIN

Moscow

MolMod DB: Molecular model database[1]

Geometry

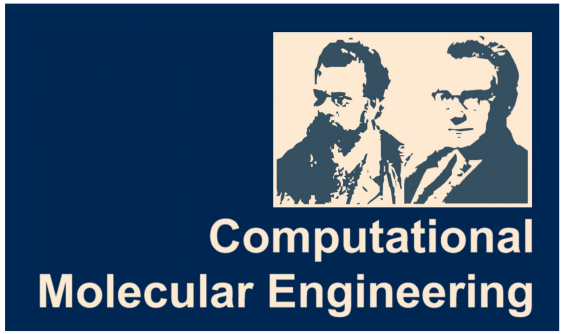
Types and positions
of interaction sites

Dispersion and repulsion

Lennard-Jones or Mie potential:
Size and energy parameters

Electrostatics

Point charge or multipole
(point dipole or quadrupole):
Magnitude and orientation



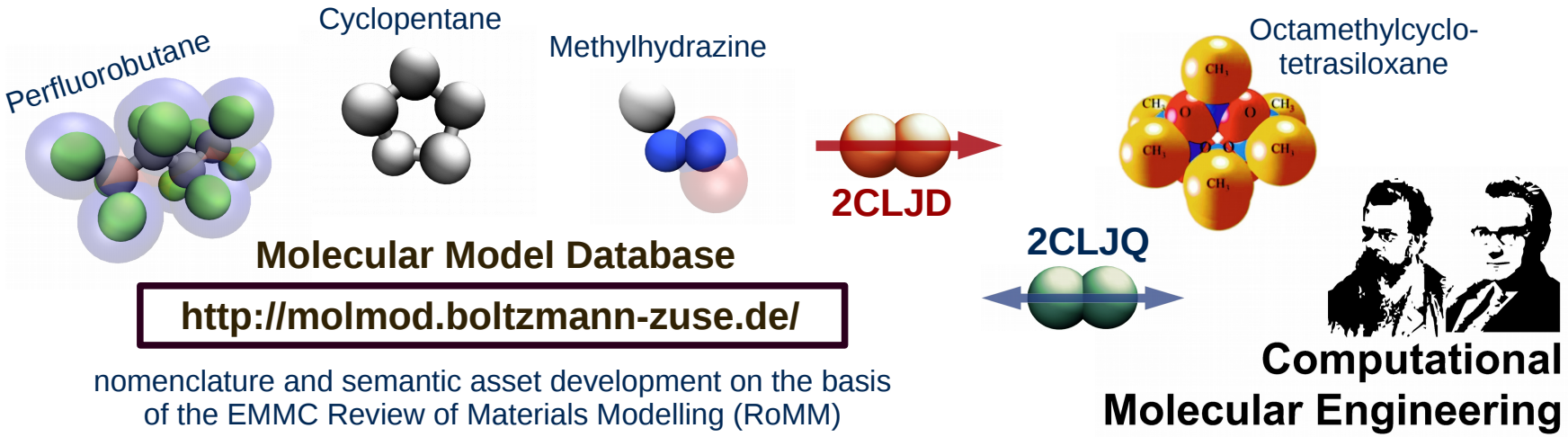
Molecular Model Database (MolMod DB)

http://molmod.boltzmann-zuse.de/

pair potentials for over 150 molecular fluids

[1]S. Stephan, M. Horsch, J. Vrabec, H. Hasse, *Mol. Sim.* 45(10), 806 – 814, **2019**.

Interoperability by semantic asset development



Molecular Model Database

http://molmod.boltzmann-zuse.de/

nomenclature and semantic asset development on the basis of the EMMC Review of Materials Modelling (RoMM)

Computational Molecular Engineering

FAIR principles of data technology

Make all data …

F INDABLE,
A CCESSIBLE,
I NTEROPERABLE,
R EUSABLE.

EMMC

EMMC Taxonda Dashboard

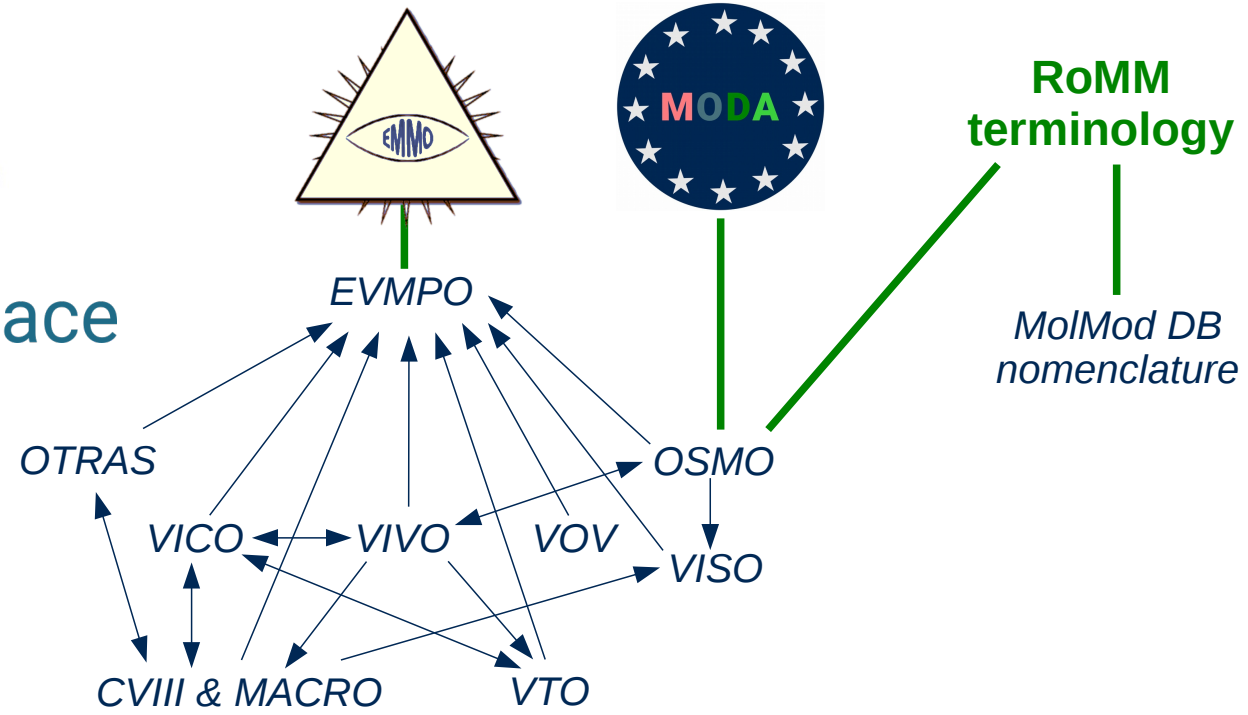
RDA Task Groups

Materials Ontologies
Semantic Assets for Materials Science

RESEARCH DATA ALLIANCE

http://rd-alliance.org/

Interoperability by semantic asset development



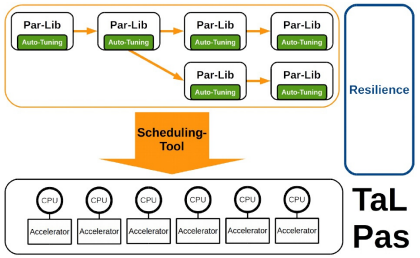
EMMC line of semantic asset development:

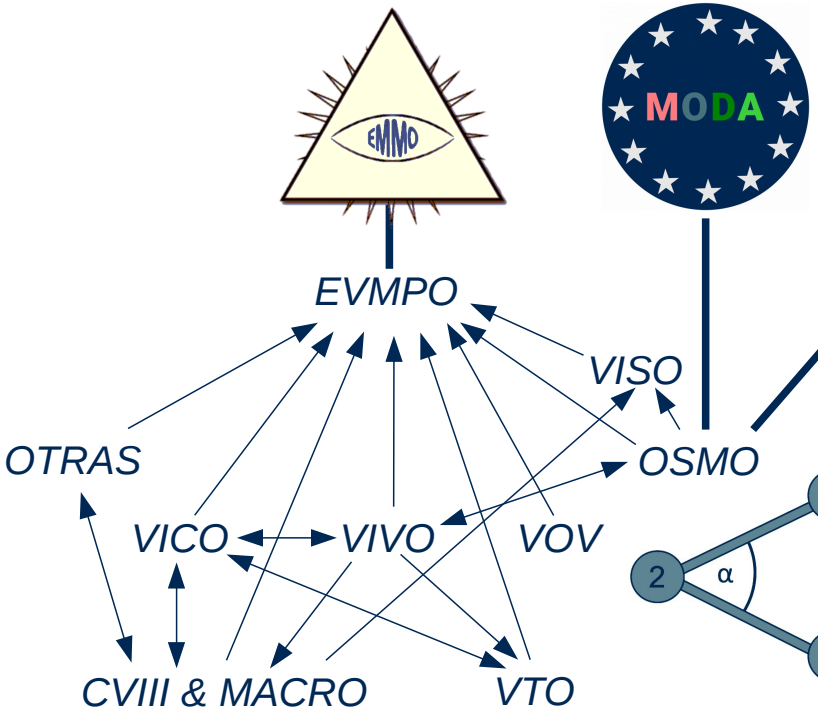
1) **Review of Materials Modelling (RoMM)**
2) **CWA 17284 – Model Data (MODA)**
3) **European Materials & Modelling Ontology (EMMO)**

Blue: Semantic assets co-developed by the Virtual Materials Marketplace (VIMMP) project

MolMod database nomenclature

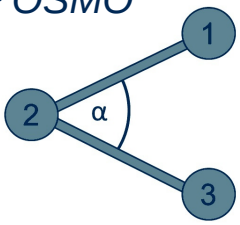
VIMMP
VIRTUAL MATERIALS MARKETPLACE

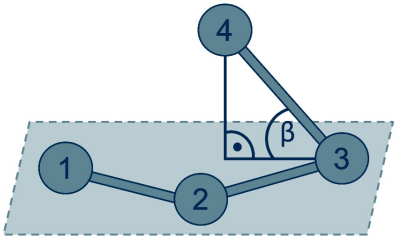




RoMM terminology

MolMod DB nomenclature[1]





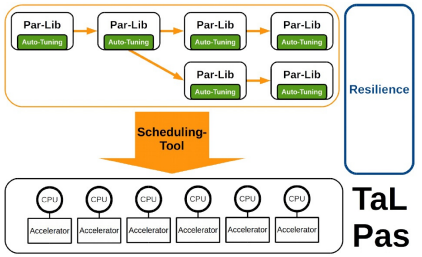
1	$name_1$	-	-	-	-	-	-
2	$name_2$	1	$distance_2$	-	-	-	-
3	$name_3$	2	$distance_3$	1	$angle_3$	-	-
4	$name_4$	3	$distance_4$	2	$angle_4$	1	$dihedral_4$
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
n	$name_n$	n-1	$distance_n$	n-2	$angle_n$	n-3	$dihedral_n$

Z-matrix formalism for the site coordinates of multi-site models[1, 2]

[1] S. Stephan, M. Horsch, J. Vrabec, H. Hasse, *Mol. Sim.* 45(10), 806 – 814, **2019**.

[2] J. Parsons, J. B. Holmes, J. M. Rojas, J. Tsai, C. E. M. Strauss, *J. Comput. Chem.* 26(10), 1063 – 1068, **2005**.

Bundesministerium
für Bildung
und Forschung



Significant collaboration acknowledged:

Berlin	–	Jadran Vrabec
Kaiserslautern	–	Hans Hasse and Simon Stephan

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 760907.

This document and all information contained herein is the sole property of the VIMMP Consortium (unless specified otherwise or clear by context). Information presented herein may be subject to intellectual property rights. No intellectual property rights are granted by the delivery of this document or the disclosure of its content. Reproduction or circulation of this document to any third party is prohibited without the consent of the authors.

The statements made herein do not necessarily have the consent or agreement of the VIMMP Consortium. They represent the opinion and findings of the authors.

©2019 all rights reserved.

VIMMP
VIRTUAL MATERIALS
MARKETPLACE