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

15th October 2019
DACOMSIN
Moscow
MolMod DB: Molecular model database

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

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)

FAIR principles of data technology

Make all data …

F INDABLE,
A ACCESSIBLE,
I INTEROPERABLE,
R REUSABLE.

RDA Task Groups
Materials Ontologies
Semantic Assets for Materials Science

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

Z-matrix formalism for the site coordinates of multi-site models$^{1,2}$

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