MedeA Molecular Builder

A Collection of Tools for Building Molecules

At-a-Glance

The *MedeA*®[1] *Molecular Builder* allows you to create a wide variety of molecular models from simple organic fluid systems to coordination complexes encountered in dyes and pigments or as homogeneous catalysts used for synthesis of organic materials. The builder integrates seamlessly with other MedeA builders enabling efficient model construction for any type of materials system.

Key Benefits

Productivity - *MedeA Molecular Builder* lets you draw, use predefined templates, import from a periodic crystal model, access fragment libraries, or use SMILES strings to quickly build the structures you need.

Accuracy - Predifined templates, extensive fragment libraries, and built-in minimization & molecular dynamics to 'clean' structures each ensure that your *MedeA Molecular Builder* models are accurate.

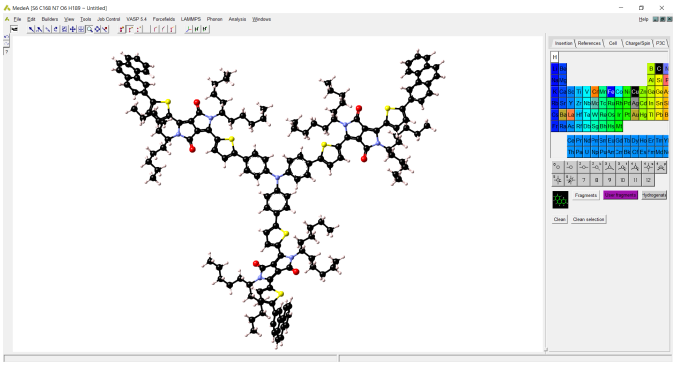
Orchestration - Use in conjunction with other *MedeA* builders to assemble complex multicomponent, multimolecular models.

Key Features

The *MedeA Molecular Builder* provides a collection of model-building tools for creating individual molecules, which will either be used directly as inputs to *MedeA*'s property calculation modules, or will be used in conjunction with other *MedeA* builders to assemble complex multicomponent, multimolecular models.

Using the *Molecular Builder* you can:

- Control the coordination and local geometry by choosing from a set of templates
- Attach complete pre-built fragments from the extensible library containing dozens of fragments of various types
  - Common aliphatic hydrocarbons
  - Aromatic and fused aromatic ring compounds
  - Fatty acids
  - Common functional groups - ethers, alcohols, halides, amines and amides etc.
  - Ligands
  - Amino acid side groups
- Generate initial coordinates using SMILES representation of the structure, or by extracting one or more molecules from a periodic model
- Transform to periodic cell representation for use with VASP and LAMMPS



'MedeA's extensive collection of builders gets you to the important part of modeling fast — namely calculating and analyzing properties of new and existing materials.'

Required Modules

- *MedeA Environment*

Related Modules

- *MedeA Amorphous Materials Builder*

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

- *MedeA Interface Builder*
- *MedeA Nanobuilder*
- *MedeA Polymer Builder*
- *MedeA Thermoset Builder*

Find Out More

Learn more about using the *MedeA Molecular Builder* by viewing the following on-line video tutorials:

- Building small molecules: How to Build a Simple Molecule
- Using the fragments library: How to Build a Complicated Molecule (MMA)
- Creating molecules from a SMILES string: How to Import from SMILES

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