MedeA Nanobuilder

"There's plenty of room at the bottom!"

Synthetic chemistry methods and analytical devices are becoming increasingly powerful. As this happens, building and manipulating nanoscale structure models, and assembling individual atoms and molecular groups represents an essential and important step in constructing physically descriptive model systems.

At-a-Glance

With the *MedeA* ®[1] *Nanobuilder*, you construct nanometer-sized atomistic models using a comprehensive set of structural building parameters. Start from simple bulk or surface slab models, select from a list of intuitive design criteria, and build sophisticated nanoscale models within minutes!

Key Benefits

- Expands the reach of atomistic simulations to include complex nanoscale assemblies
- Seamlessly integrates with other *MedeA* Builders, *MedeA* workflows, and *MedeA* compute engines

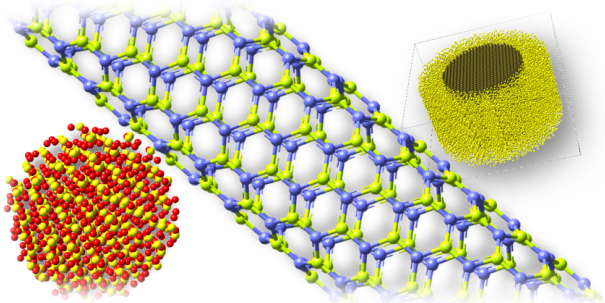

Figure 1: MedeA Nanobuilder*: user-friendly builder for nanoparticles, nanotubes, and nanowraps*

The MedeA Nanobuilder lets you transform crystal structures into nanospheres or nanocylinders easily. Or, construct various types of single-wall or multi-wall nanotubes or nanowraps, all with just a few mouse clicks. Nanobuilder output is passed directly to the *MedeA Molecular Builder* where you may further edit the structure, e.g. by adding functional groups, or pacifying by passivating dangling bonds.

Key Features

- Interactive GUI-based Builder
- Intuitive design criteria guiding construction
  - sphericity, chirality, rotation axes, nesting
- Nanoparticles: spherical, cylindrical
- Nanotubes: single wall, multiwall, nested, armchair, zigzag
- Nanowraps: torus-shaped like layers and wraps
- Control of dangling bonds

'There's plenty of room at the bottom'

Richard Feynman, 1959

MedeA Nanobuilder in Action

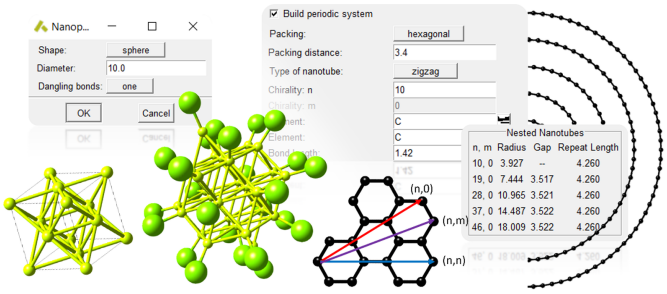

Figure 2: MedeA Nanobuilder *screenshots: building spherical nanoparticles, controlling bond passivation, designing single-wall and nested multi-wall carbon nanotubes*

Required Modules

- *MedeA Environment*

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

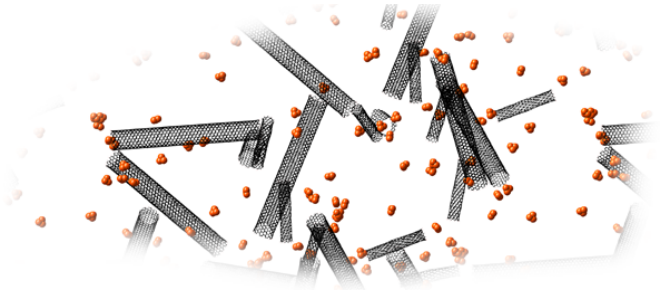

Figure 3: MedeA Nanobuilder *integration with Amorphous Builder: nanotubes in solution*

Supported Modules

- *MedeA LAMMPS*
- *MedeA VASP*
- *MedeA MOPAC*
- *MedeA GAUSSIAN*
- *MedeA Molecular Builder*
- *MedeA Polymer Builder*
- *MedeA Amorphous Materials Builder*

Find Out More

Learn more about *MedeA* features and capabilities: Databases, Builders, Compute Engines, Forcefields, Property Modules, Analysis Tools, and High-Throughput.

Watch our Upcoming and Recorded Materials Design webinars on *MedeA* for related topics in computational materials design and materials engineering.

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