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# Polymer Builder

**Version:** Q-2019.12

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In this tutorial you will learn how to use the **Polymer Builder** to build polymers such as homopolymers and polymer blends, and how to include embedding of molecules, nanoparticles, or a surface, all using the Nanolab GUI. The Polymer Builder is introduced with the Q-2019.12 version of QuantumATK. After building the inital polymer model, you can proceed to perform realistic atomistic simulations for studies of the polymer properties such as polymer melting, glass transition temperature, mechanical properties, miscibilty, and so on.

This tutuorial guides how to build an initial polymer using the **PolymerBuilder** script block located in the **Script Generator**.

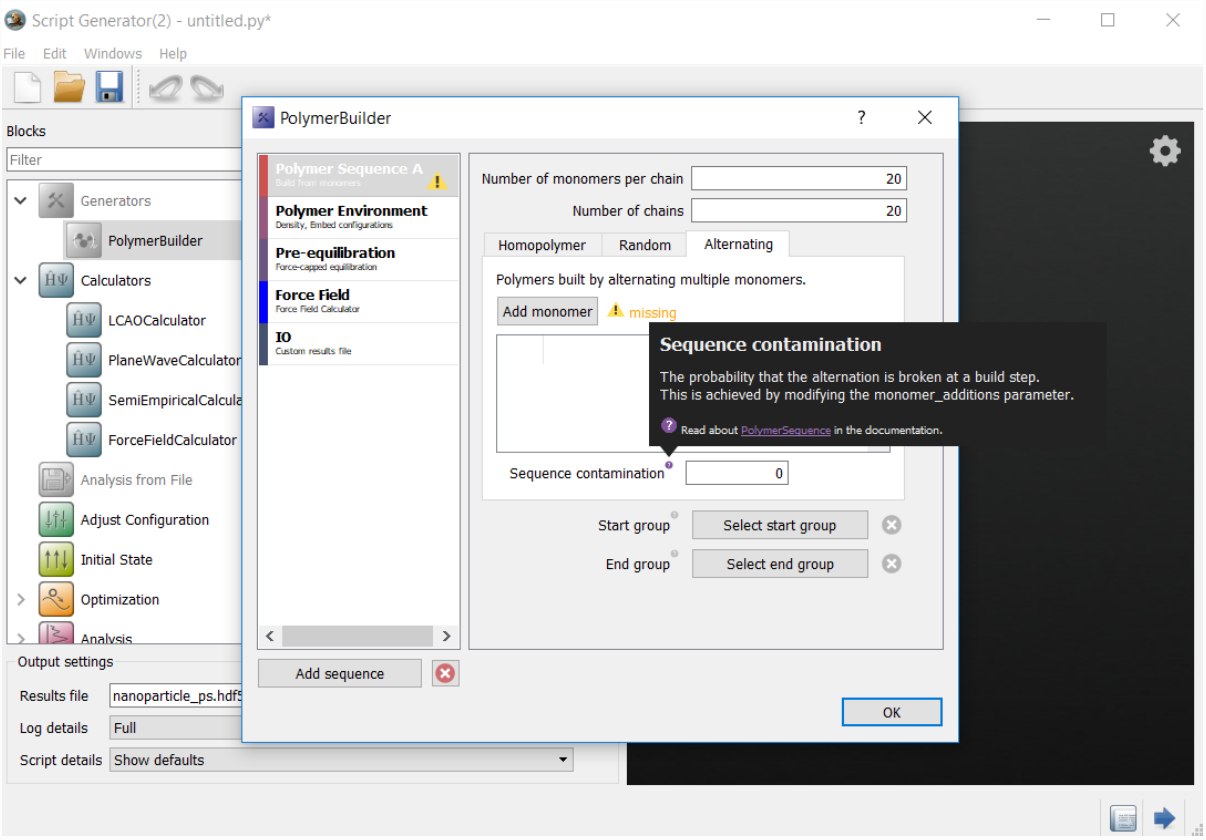
**Contents**

## Procedure of the Polymer Builder

1. Open the **Script Generator**.
2. Add the **PolymerBuilder** block under the **Generator** into the the templates.

> **Note**
>
> The **PolymerBuilder** object is located in **Script Generator** not in **Builder**. Monomers of polymer sequences are stored in the **Monomer Database** which is newly implemented in Q-2019.12. You can also create and add customized monomers into the **Monomer Database**. You will learn it in the Customized monomer section of tutorial.

3. Decide the polymer sequences. In the **Polymer Sequence A**, you see `Homopolymer`, `Random`, `Alternating`. The `Homopolymer` builds one main monomer chain, while `Random` and `Alternating` can build the polymer chains consisting more than two monomers randomly or alternatively. When you click the small question sign, you get a short description such as the below figure.




Tacticity or Sequence contamination is in a range of 0 and 1. And the number of monomer per chain and the number of chains are each 20 as a default. You can also add the different polymer sequence clicking the button of `Add Sequence`. When you select the `monomer`, `start group`, or `end group`, **Monomer Database** will be pop-up automatically.

4. In the **Polymer Enviroment**, you can set up the polymer density and embeded host configuration and molecules. PolymerBuilder builds melted polymer with a defined density controlling a periodic box size. But in the embedded case with a host configuraiton, polymers are packed in the periodic box of host configuration. And many applications include not only polymer, but also nanoparticles, surfaces or molecules. You can setup to build polymer with embedded other material types.
5. **Polymer Monte Carlo** `PolymerMonteCarloBuilder` runs with above defined conditions.
6. **Pre-equilibration** is performed after Polymer Monte Carlo. It is using the **Force-Capped Molecular**

**Dyanmics** `ForceCappedMolecularDynamics`. Initial configuration by Polymer Monte Carlo includes overlapped atoms or artifically closed atoms. Optimization and Force-capped molecular dynamics run to make a reasonable configuration.

7. PolymerBuilder runs by `Dreiding` or `OPLS` force field. The desired polymer system should be parameterized in `Dreiding` `DreidingPotentialBuilder` or `OPLS` `OPLSPotentialBuilder` force field types.
8. Run it using the **Job manager**. Polymer is usually much larger than molecular/bulk system. Due to the number of atoms and scale of size, it takes a bit longer time, especially for the pre-equilibrium step.

## Homopolymer

You will build *polyvinylidene fluoride (PVDF)* polymer as an example.

- Open the **PolymerBuilder**.
- In the **Polymer Sequance A**, see `Homopolymer`. You can create a polymer model from a single monomer in this section.
- Click the `Select monomer` to load the monomer. It is pop-up the **Monomer Database** which includes common monomers.
- Select `tetrafluroethylene` to build the *polyvinylidene fluoride (PVDF)*. There is an option to define the tactic ratio. `Isotactic` is `0` and `Syndiotactic` is `1`. Default is `Atatic` with `0.5` ratio of isotactic and syndiotactic. You can also customize the atatic ratio in the `Custom`.
- Move to the **Polymer Environment**. You can set the desired density with a unit of g/cm $^3$. Change the density into `1.78` g/cm $^3$ in experiment for *PVDF*.

You can also see the **Pre-equilibration** section. After generating an initial polymer model by Polymer Monte Carlo, PolymerBuilder follows the pre-equilibration using the Force-capped equilibration method. It is for preventing the overlapping or artifically closed atoms. Detailed information is documented in the manual page, `ForceCappedEquilibration`. You will keep the default condition for others.

- Change the output file as `pvdf.hdf5` and open the **Editor** to confirm the settings as an input script.

You can see the following information in the input python file.

The first part of script shows the definition of monomer configuration as *MoleculeConfiguration* with information of tags and bonds using the `Dreiding` or `OPLS` force field. QuantumATK PolymerBuilder includes the `Dreiding` or `OPLS` force field. The `Dreiding` force field is much simpler than `OPLS` force field. PolymerBuilder can automatically indicate the types of `Dreiding` force field. Therefore, when you use `Dreiding` force field, you don't need to add the tags manually. But it is too simple not to describe the tacticity or partial charge. On the other hand, the `OPLS` force field is able to consider the tacticity and partial charge of atomic types. It is more complex but more accuracy. You can use it adding tags connected to the `OPLS` parameters for monomer configuration.

PolymerBuilder uses the `Dreiding` and `OPLS` force field parameters to build a polymer model using the Polymer Monte Carlo and Force capped equilibration.

In the following section as shown in the below script, polymer Monte Carlo builder is defined. After building an initial polymer, pre-equilibration will be performed using the force capped equilibarion method. Force capped equilibration will run 4 cycles. Each simulation runs 40,000 times with 0.5 fs timestep as a default. The `OPLS` potential is used in Force capped equilibration.

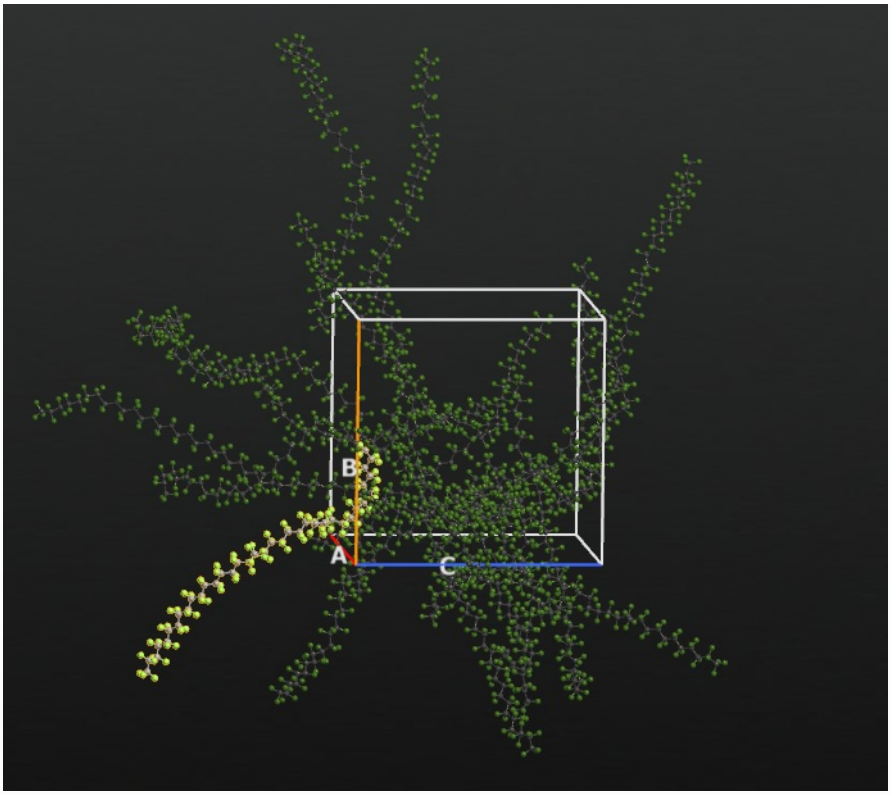
```
# ------------------------------------------------------------
# Polymer Monte Carlo Builder
# ------------------------------------------------------------
polymer_builder = PolymerMonteCarloBuilder(
    polymer_sequence=polymer_sequences,
    density=1.7800*gram/cm**3,
    monte_carlo_temperature=300.0*Kelvin,
    angle_sampling_points=20,
    repack_molecules=False,
    )
bulk_configuration = polymer_builder.buildPolymerConfiguration()

# ------------------------------------------------------------
# Calculator for Force Capped Equilibration
# ------------------------------------------------------------
potential_builder = DreidingPotentialBuilder(
    include_electrostatic=False,
    )
calculator = potential_builder.createCalculator(bulk_configuration)
bulk_configuration.setCalculator(calculator)

# ------------------------------------------------------------
# Force Capped Equilibration
# ------------------------------------------------------------
equilibration_method = ForceCappedEquilibration(
    temperature=300.00*Kelvin,
    md_steps_per_force_capped_simulation=40000,
    md_time_step=0.50*fs,
    force_capped_simulations=4,
    starting_factor=1.040,
    ending_factor=0.800,
    fixed_indices=None,
    )
bulk_configuration = equilibration_method.runEquilibration(bulk_configuration)
nlsave('pvdf.hdf5', bulk_configuration)

# ------------------------------------------------------------
# Calculator
# ------------------------------------------------------------
potential_builder = OPLSPotentialBuilder(
    lennard_jones_cutoff=10.0*Angstrom,
    electrostatic_accuracy=0.0001,
    )
calculator = potential_builder.createCalculator(bulk_configuration)
bulk_configuration.setCalculator(calculator)
nlsave('pvdf.hdf5', bulk_configuration)
```

Now you are ready to run the script. Go to the **Job manager** after saving the script as `pvdf.py`. It takes around 15 minutes on your laptop.

After the job finishes, you can visualize the results using the **Viewer**. .. , when you select the `pvdf.hdf5`, .. you can see 2 objects of `BulkConfiguration_0` and `BulkConfiguration_1` .. on the **labfloor**. .. `BulkConfiguration_0` is the configuration after polymer Monte Carlo .. and `BulkConfiguration_1` is the configuration after pre-equilibration process. .. You can compare them in the **Compare Configurations** plug-in. .. You can also visualize it using the **Viewer**.

As shown in the below figure, you can see the 20 chains with 20 monomers per each chain of *PVDF* with `1.78` g/cm $^3$ density. The periodic box is automatically controlled to fit the requested density.

You may need to increase the *Fuzz factor* (ex. `1.15`) in the **Graphics Properties** of **Viewer** to see reasonable polymer chains. And the default configuration shows unwrapped configuration. When you check the *wrap atom*, you can see the wrapped configuration in a periodic box.




## Polymer blend

Pactically, polymer blend is important to mix different polymers. You can easily build the polymer blend using the **PolymerBuilder**. We will blend *Poly Methyl Methacrylate (PMMA)* and *Poly Vinyl Chloride (PVC)* in a periodic box as an example.

- Open the **PolymerBuilder**.
- Click `Add sequence` in the botton side of **PolymerBuilder** widget.

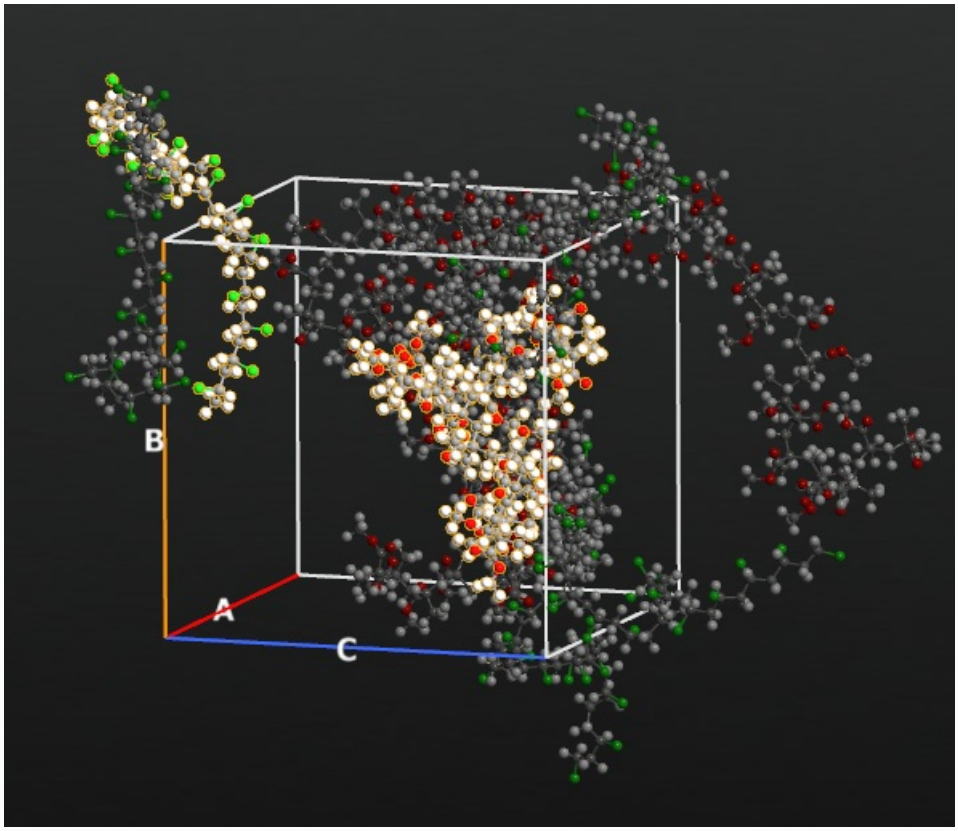
Now you can make two different polymer sequences. If you need more different polymer sequence, you can add it more from here.

- In the **Polymer Sequance A**, select the `Methyl Methacrylate` in the Monomer Database.
- In the **Polymer Sequance B**, select the `Vinyl Chloride` in the Monomer Database.

To demonstrate it in a short time, you will blend simply two different polymers of 5 chains possessing 20 monomers per chain.

- Change the number of chains into `5` in the Polymer Sequance A and B.
- Change the output file name as `pmma-pvc.hdf5`. Other options are default.
- Open the **Editor**. You can see molecular configuration and parameters of 2 monomers from polymer sequence a and b in the script.
- Save the script as `pmma-pvc.py` and run it in the **Job Manager**.

It takes around 20 minutes in your laptop. As shown in the following figure, you get the polymer blend system including 5 *PMMA* and 5 *PVC* chains.




## Polymer with embedded molecules

In many cases, polymer is melted in liquid. The tutorial guides how to embed molecules into the polymer, as building the *PMMA* polymers with methane molecules as a simple example.

It starts with one monomer and one molecule.

- In the **Polymer Sequance A**, select the `Methyl Methacrylate` in the Monomer Database. And change the number of chain as `5`.
- Open the **Builder** and import `Methane` **From Database** of Molecules.
- In the **Polymer Environment**, click `Add molecule from file` button.

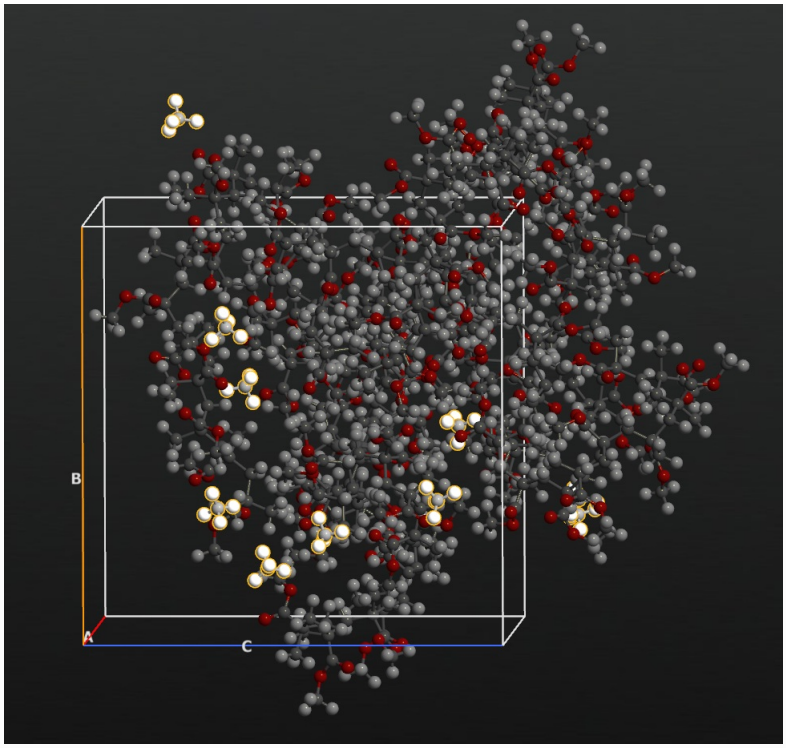
You see saved configurations in your project and also see *MoleculeConfiguration Methane* in the `Builder_Stash.hdf5`.

- Select *MoleculeConfiguration Methane* and modify `Count` as `10`.
- In the **Force Field**, change `OPLS` into `Dreiding` force field. Because the new embedded methane will run using the Dreiding force field without assigning the OPLS tag for methane manually.
- Save the output file as `pmma_methane.hdf5`.
- Open the **Editor** and confirm the script.

Embedded molecules are defined as called *Included Molecule 1* with configuration and bonds information in the polymer Monte Carlo builder. In this condition, 5 *PMMA* chains will be generated by embedded 10 *Methane* molecules.

- Run the job in the **Job Manager**.

It takes around 15 minutes on the laptop. You can see 5 chains of *PMMA* and 10 methanes in a periodic box as shown in the below figure.




## Nanoparticles in a melted polymer

There are two ways to embed nanoparticles in a melted polymer system.

1. Embed nanoparticles as a host configuration. The host configuration will be fixed during the polymer Monte Carlo and force capped molecular dynamics. Therefore polymer will be positioned in space defined by the host configuration.
2. Embed nanoparticles as molecules. Smaller sized nanoparticle can be assumed as molecules. You can load a nanoparticle from `Add molecule from file`. Such as embedded molecules Polymer with embedded molecules, you can also add how many particles will be embedded. In this case, embedded nanoparticle configuration should be a type of `MoleculeConfiguration`. And it is randomly positioned with polymers by Polymer Monte Carlo.

In this tutorial, you will embed about `15` Å sized *Silica* nanoparticle with *poly-stylene* polymer.

You will firstly embed a nanoparticle using the host configuration.

**Note**

The host configuration is fixed, while polymers are generated into the host configuration by polymer Monte Carlo builder. You can import and embed any kinds of host configuration with polymers.

Polymer Monte Carlo is parameterized by `Dreiding` or `OPLS` force fields. Considering atomic types should be able to use in `Dreiding` or `OPLS` force field parameter.

- Open the **PolymerBuilder**.
- In the **Polymer Sequance A**, select the `Stylene` in the Monomer Database. And change the number of chains as `10`.
- In the **Polymer Environment**, click `Add bulk from file` button.

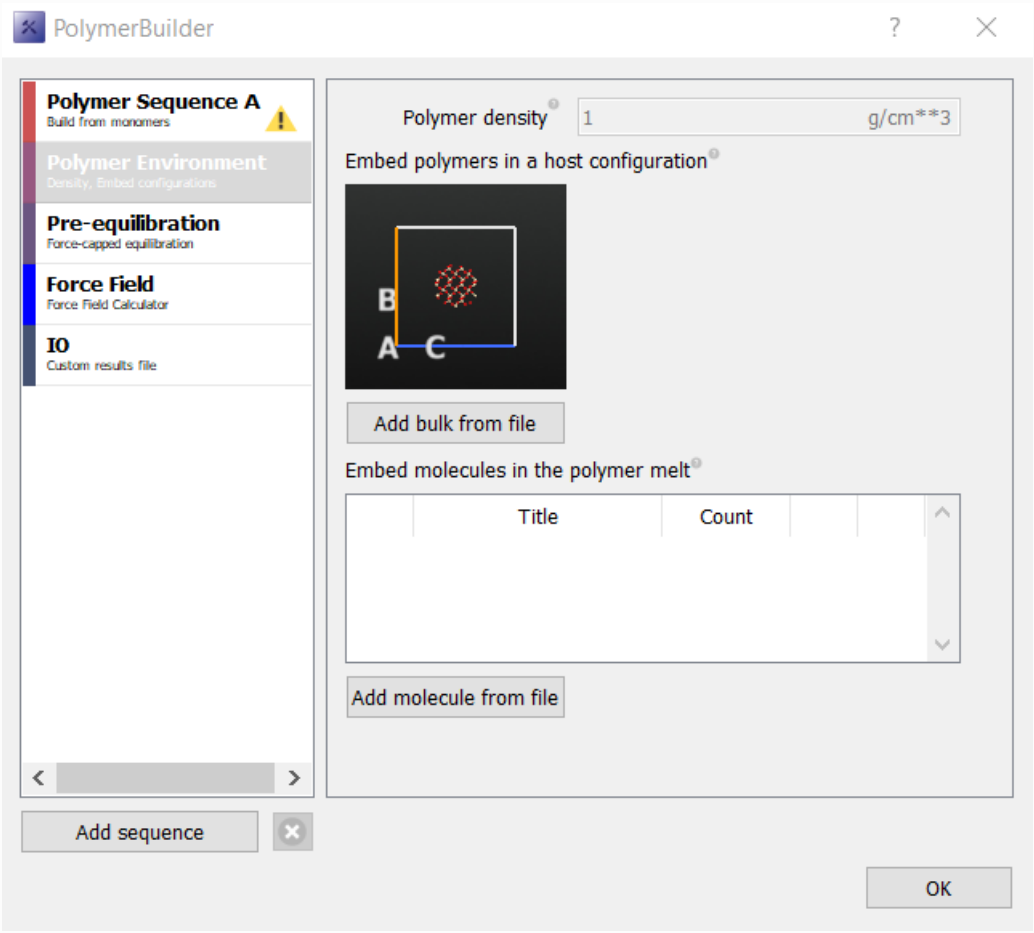
You see saved configurations in your project. Import the host configuration here. In this tutorial, download the `15` Å sized $SiO_2$ nanoparticle configuration in a `35` Å x `35` Å x `35` Å periodic box,

sio2_nanoparticle.hdf5 and use it.

**Note**

Once you use the host configuration selecting the `Add bulk from file`, `polymer density` is inactive because polymer is packed in the defined periodic box of host configuration.

- Select the `BulkConfiguration_0` of `sio2_nanoparticle.hdf5`. You can see the host configuration on the widget as the below figure.




- In the **Force Field**, change `OPLS` into `Dreiding` force field. Because the new embedded nanoparticle will run using the Dreiding force field without assigning the OPLS force field manually and in the case of $SiO_2$ nanoparticle, OPLS will be in a trouble not to make a neutral charge in a total configuration.
- Save the output file as `host_nanoparticle_10ps.hdf5`.
- Open the **Editor** and check the script.

You can see *Host configuration information*.

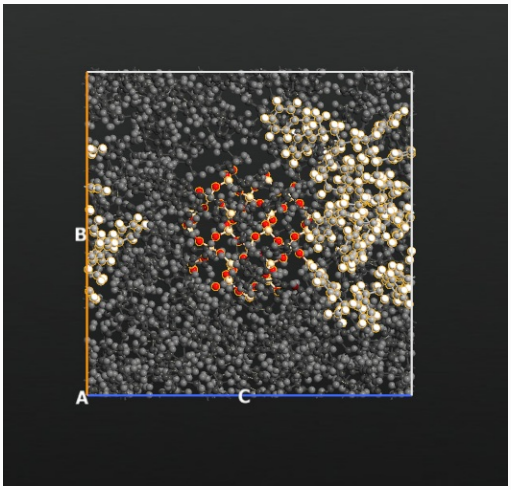
- Run the job after saving the input file as `host_nanoparticle_10ps.py`.

It takes around 30 minutes on the laptop.

**Note**

Once the host configuation is large, it takes time to build it even in the MPI process. Polymer builder by polymer Monte Carlo takes a few minutes in your laptop, but force capped molecular dynamics takes time depending on the number of atoms. Such a large system probably needs more steps than default in pre-equilibration to have a reasonable configuration.

The configuration of $SiO_2$ nanoparticle with 10 *PS* is shown in the below figure.




You will now build nanoparticles in polymer as the embed molecules.

- Open the **PolymerBuilder**.
- In the **Polymer Sequance A**, select the `Stylene` in the Monomer Database. And change the number of chains as `10`.
- In the **Polymer Environment**, click `Add molecule from file` button.

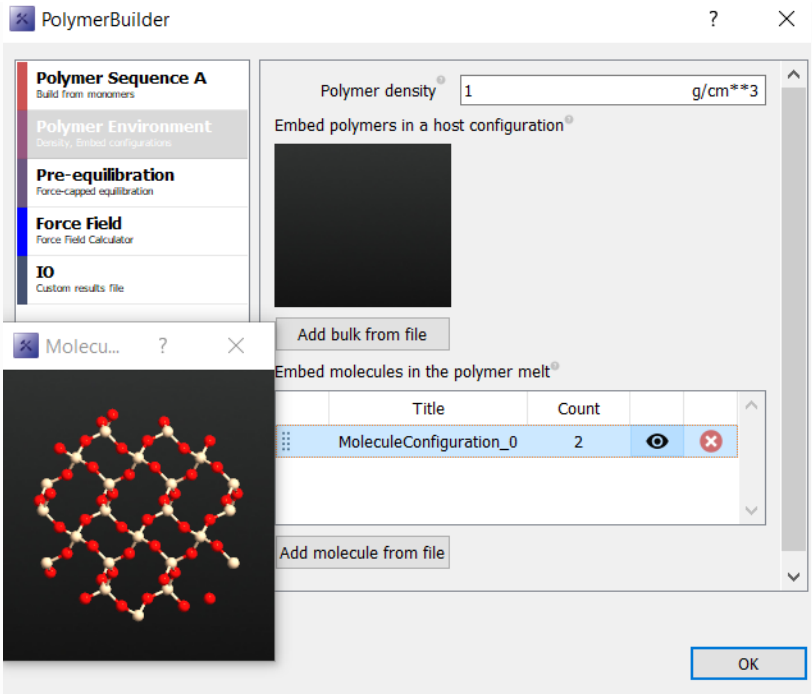
You see saved configurations in your project. But unlike the host configuration, you need a molecular type of configuration.

- Open the downloaded sio2_nanoparticle.hdf5 in the **Builder**.

It is the `15` Å sized $SiO_2$ nanoparticle configuration in a `35` Å x `35` Å x `35` Å periodic box. We will remove the periodic box and save as a MolecularConfiguration.

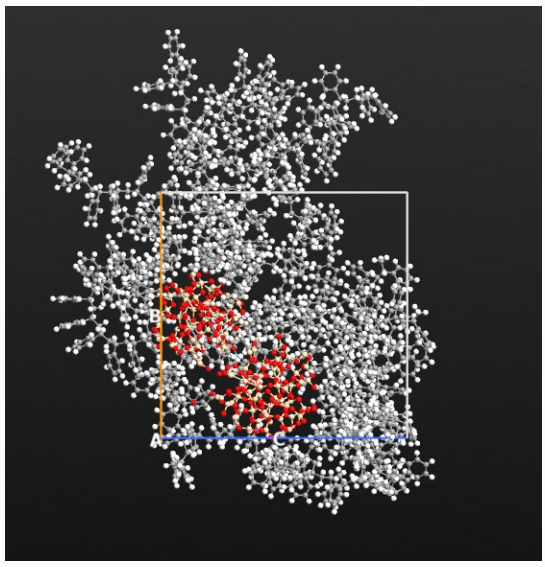
- Change the current configuration into a molecule configuration clicking the icon.
- Save the configuration as `sio2_nanoparticle_molecule.hdf5`.
- Now when you click `Add molecule from file` button again, you see it including `MoleculeConfiguration`.
- Load the `MoleculeConfiguration` in `sio2_nanoparticle_molecule.hdf5`.
- In this case, you will embed 2 nanoparticles. Change the `Count` into `2`.

As the below figure, you can visually check the embed nanaparticle configuration and the number of particles.




- In the **Force Field**, change `OPLS` into `Dreiding` force field. Because you will not assign the OPLS force field on the nanoparticle manually.
- Save the output file as `2nanoparticle_10ps.hdf5`.
- Open the **Editor** and check the script.
- Run the job after saving the input file as `2nanoparticle_10ps.py`.

It takes around 30 minutes on the laptop. As shown in the following figure, 2 nanoparticles are randomly positioned with polymers. In this case, it is fit to the defined polymer density controlling the periodic box. And nanoparticles and polymers are relaxed by pre-equilibration process.



## Polymers around a surface

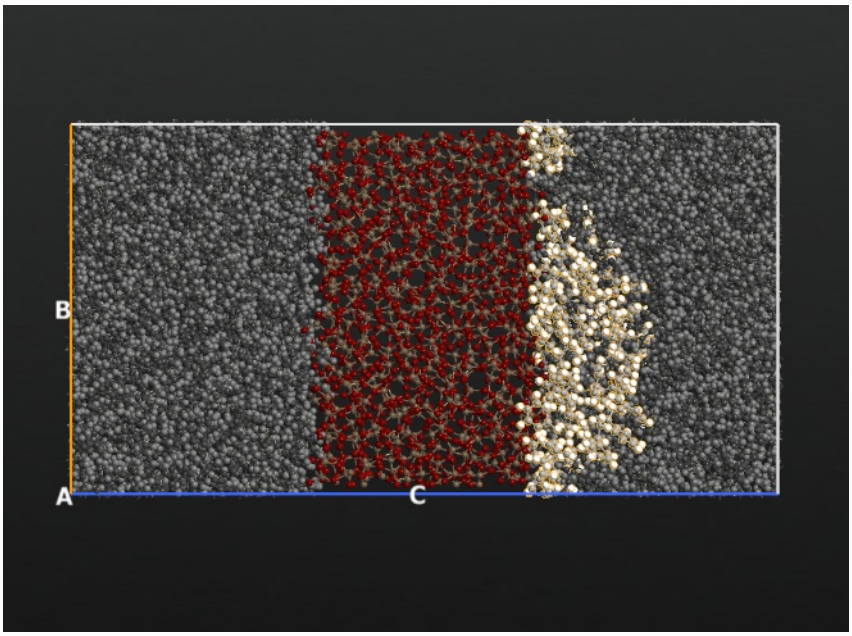
Now you will see an advanced example using the *Poly-stylene* melt with amorphous OH-terminated $SiO_2$ surface. It is a same procedure to use a host configuration to import the surface configuration as shown in the nanoparticle example. Download the OH-terminated amorphous $SiO_2$ surface configuration, sio2_surface.hdf5 and use as a host configuration.

You will build 20 *poly-stylene* chains of 40 monomers per chain with embedded OH-terminated $SiO_2$ amorphous surface configuration with `25` Å thickness of $SiO_2$ in about `40` Å x `40` Å x `80` Å sized

periodic box as a host configuration.

During the polymer Monte Carlo, the host configuration is fixed to generate 20 *poly-stylene* in a periodic box. After that, Force-capped molecular dynamics will be performed by force field parameters.

It has more than 16,000 atoms. Generation of random polymers by polymer Monte Carlo takes a few minutes on the laptop. But the force-capped molecular dynamics takes a quite long time even in the default condition. Probably you need more steps to get a reasonable configuration in the pre-equilbrium. The below figure shows the 20 *Poly-stylene* melt with amorphous OH-terminated $SiO_2$ surface with highligted one chain of *Poly-stylene*.




## Customized monomers

The Monomer Database of QuantumATK includes several types of monomers. But you may need to design and save customized monomers. You can add customized monomer into the Monomer Database in `/.vnl/databases/monomers` of user home directory.

Original shipped QuantumATK Monomer Database is located in the `/share/nanolab/monomers` of installer directory. You will see some grouping directories such as `Condensation_Monomers`, `Endgroups`, or `Vinyl_Monomers`. When you open one of monomer database (ex. `Tert-Butyl Methacrylate.py`), you see the configuration information with tags. *Add tags* include the information of atom type in a monomer such as `END`, `HEAD`, `TAIL`, `CONNECT`, `GROUP_A` and so on. You can design your own monomer. And add tags and bonds with a correct format and save the python file in `/.vnl/databases/monomers` of user home directory.

We guide the simple way to modify the monomer. This tutorial demonstrates to add `OH` functional group in the `Tert-Butyl Methacrylate` monomer.

In the `/share/nanolab/monomers/Vinyl_Monomers`,

- Drag the `Tert-Butyl Methacrylate.py` into **Builder**.

You see the `Tert-Butyl Methacrylate` monomer on the window.

- Open the *Tags* in the **Selection Tools** plug-in.

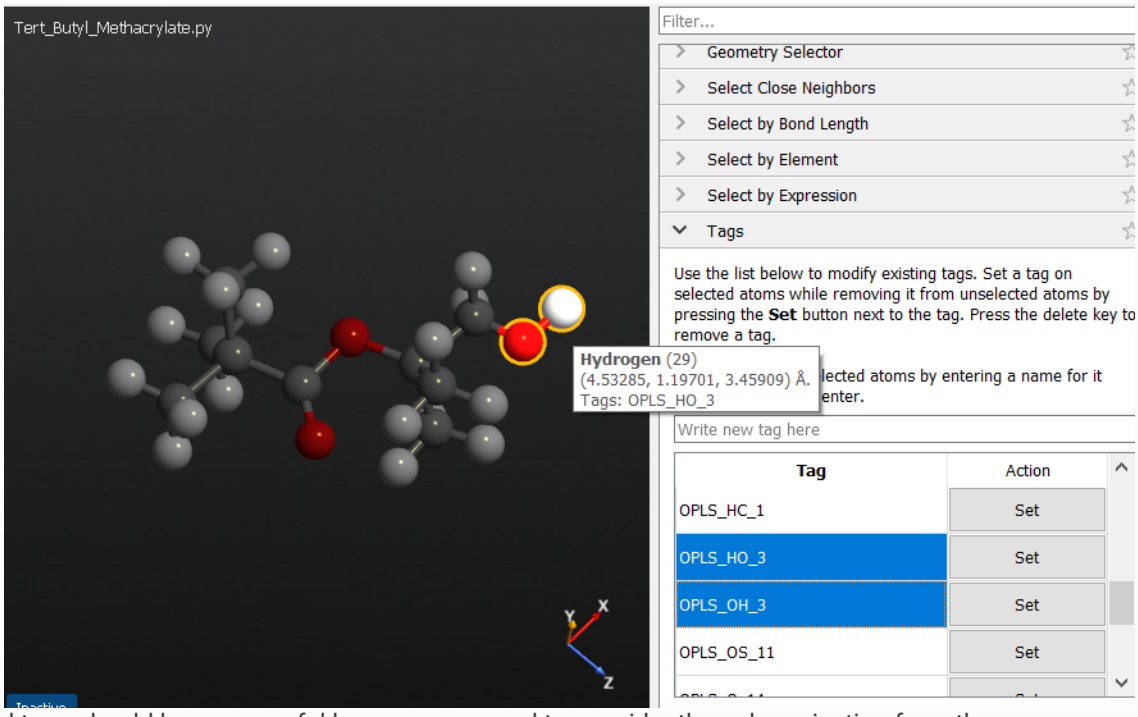
You can see the existed tags of `Tert-Butyl Methacrylate` monomer. When you choose one of tags, atom selection will be together. Acoording to this tags, for instance, `HEAD_GROUP_A` and `TAIL_GROUP_A` will finally overlap to formate the polymer. You will modify one of hydrogens not to be effect on the formation of main polymer chain.

- Change `Hydrogen` of atom number `23` into `Oxygen` atom.
- Click the icon of passivate the configuration with hydrogen.

You will see the `OH` group instead of hydrogen. You need to define the atomic parameter using the `Dreiding` or `OPLS` force field.

- Write new tag in Tags plug-on tool such as O (atom number `23`) into `OPLS_OH_3`, new H (atom number `29`) into `OPLS_HO_3`. And remove or modify the previous tags for OH functional group. For instance, remove the changed hydrogen (atomic number `23`) in `OPLS_HC_1` tags and modify the carbon (atom number `11`) attached OH group into `OPLS_CT_11` tag.

It is shown in the below figure.




Add tags should be very careful because you need to consider the polymerization from the monomer. Otherwise force field type is not correct. You can see in detail the Dreiding and OPLS potential parameters of QuantumATK in the `DreidingPotentialBuilder` and `OPLSPotentialBuilder`.

**Note**

ATKPython has functions of `DreidingPotentialBuilder` and `OPLSPotentialBuilder` that tell the types that you have, and gives a short description of them. Try the function `printTotalTypes()` on the `DreidingPotentialBuilder` and `OPLSPotentialBuilder`. It gives a table for all of the available types. Monomers should have the right tags, then they work with it.

- Open the script using the **Editor** in the Send to.

You will see new tags with `OPLS_OH_3` for atom number `23`, `OPLS_HO_3` for atom number `29`, `OPLS_CT_11` for atom number `11`. And you also add bond information. Atom number `29` needs to make a new bond with atom number `23`. You should add it with the format of *Add bonds*.

```
# Add tags
monomer_1.addTags('ENDH_OPLS_CT_4', [0])
monomer_1.addTags('HEAD_CONNECT',   [0])
monomer_1.addTags('HEAD_GROUP_A',   [1])
monomer_1.addTags('H_C',            [20, 21, 22, 24, 25, 26, 27, 28])
monomer_1.addTags('OPLS_CT_11',     [11])
monomer_1.addTags('OPLS_CT_4',      [9, 10, 12, 16])
monomer_1.addTags('OPLS_CT_5',      [0])
monomer_1.addTags('OPLS_CT_8',      [4])
monomer_1.addTags('OPLS_CT_95',     [8])
monomer_1.addTags('OPLS_C_19',      [5])
monomer_1.addTags('OPLS_HC_1',      [ 1,  2,  3, 13, 14, 15, 17, 18, 19, 20, 21, 22, 24,
                                     25, 26, 27, 28])
monomer_1.addTags('OPLS_HO_3',      [29])
monomer_1.addTags('OPLS_OH_3',      [23])
monomer_1.addTags('OPLS_OS_11',     [6])
monomer_1.addTags('OPLS_O_14',      [7])
monomer_1.addTags('TAIL_CONNECT',   [4])
monomer_1.addTags('TAIL_GROUP_A',   [16])
monomer_1.addTags('TAIL_GROUP_B',   [12])

# Add bonds
bonds = [[ 0,  1],
         [ 0,  2],
         [ 0,  3],
         [ 0,  4],
         [ 4,  5],
         [ 4, 12],
         [ 4, 16],
         [ 5,  6],
         [ 5,  7],
         [ 6,  8],
         [ 8,  9],
         [ 8, 10],
         [ 8, 11],
         [ 9, 26],
         [ 9, 27],
         [ 9, 28],
         [10, 20],
         [10, 21],
         [10, 22],
         [11, 23],
         [11, 24],
         [11, 25],
         [12, 13],
         [12, 14],
         [12, 15],
         [16, 17],
         [16, 18],
         [16, 19],
         [23, 29]]
monomer_1.setBonds(bonds)
```

- Save the new monomer with new tags as `Custom_Tert_Butyl_Methacrylate.py` creating the new directory as `Custom` in the `/.vnl/databases/monomers` of user home directory.

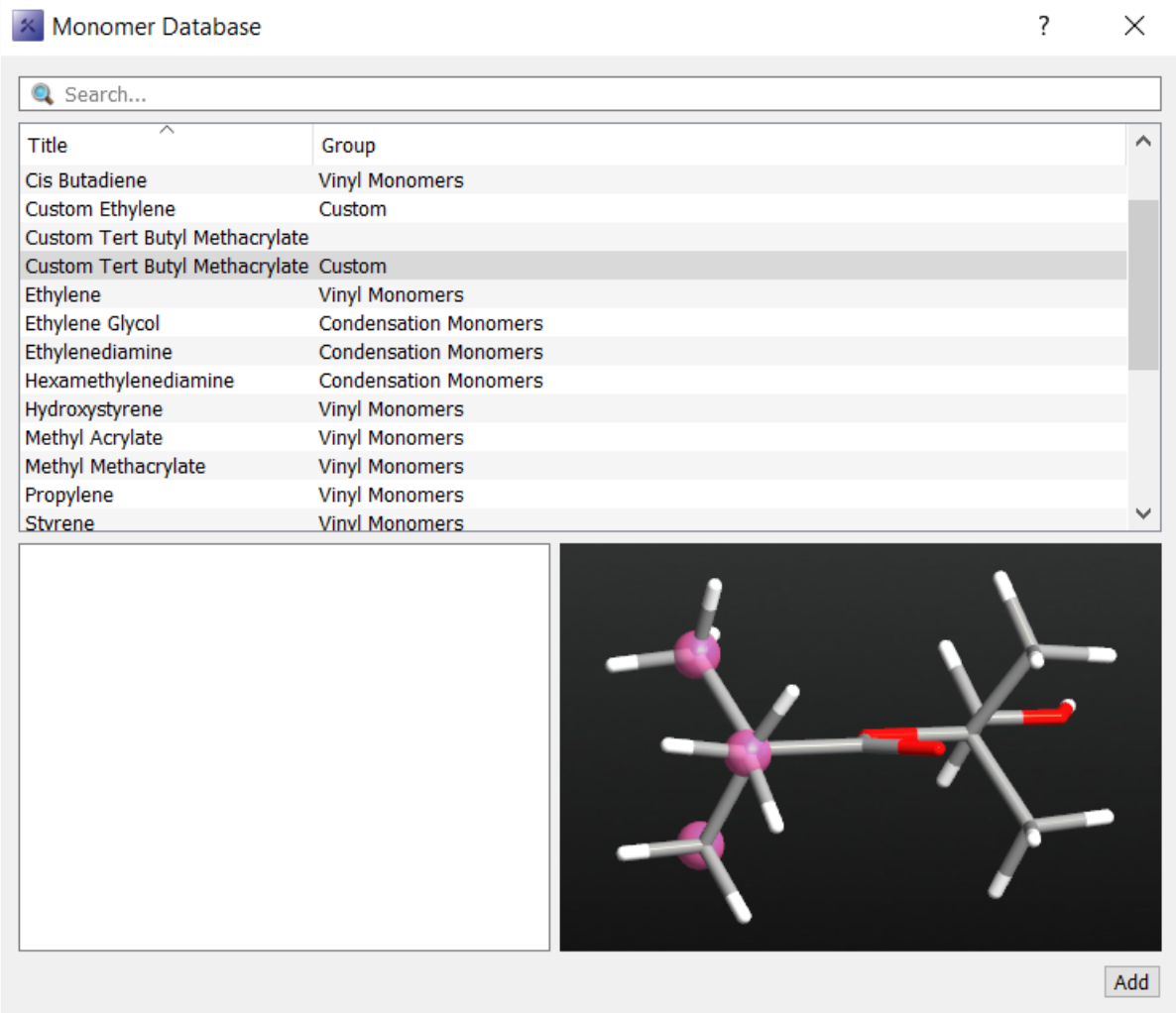
**Note**

If you create a new directory in `/.vnl/databases/monomers`, it will make a grouping with the directory name. After creating a new monomer by user, you need to restart the **Script Generator**.

Now you can load the customized monomer from the Monomer Database in the PolymerBuilder GUI.

- Open the PolymerBuilder.
- Click the `Select monomer`.

Now you see the `Custom Tert Butyl Methacrylate` in the momoner database as the below image. When you click it, you also see the configuration indicating how to connect the main chain and `OH` functional group on the widget.

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