Integrating Industry Standard Rendering Techniques for Visualizing Solvation in Molecular Dynamics Simulations Using The MolecularNodes Software Plug-in

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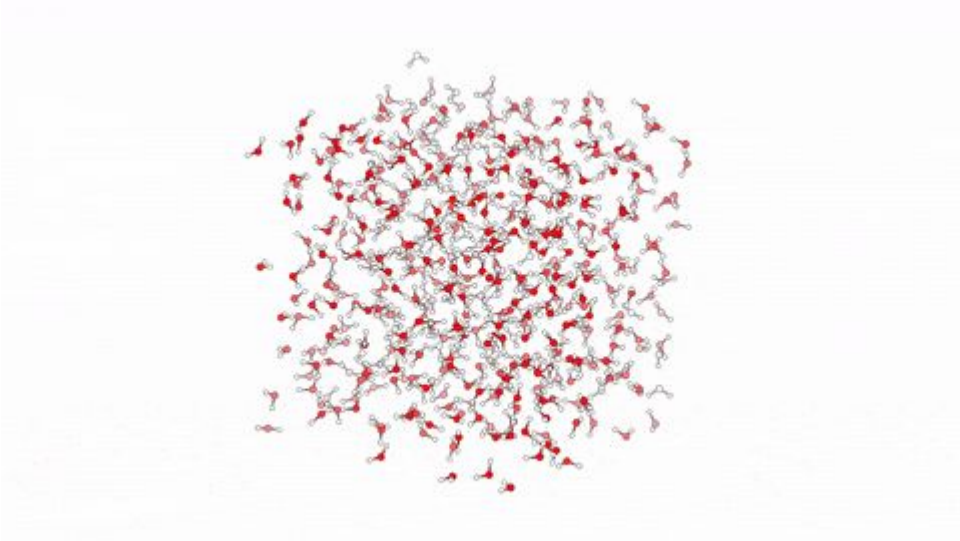
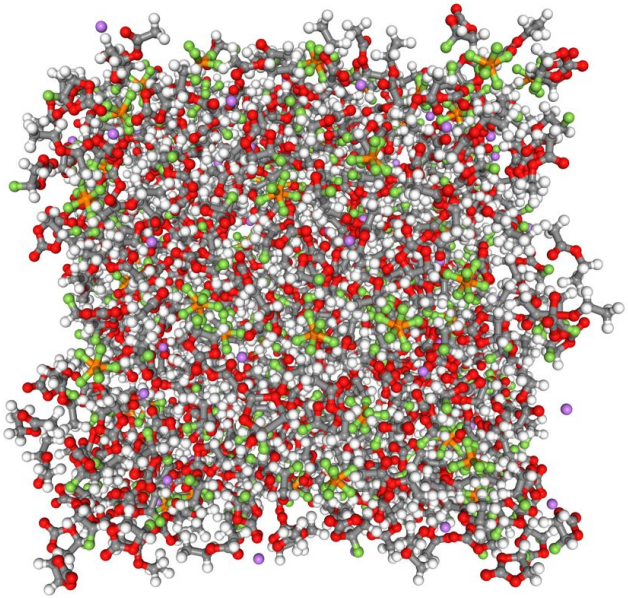
BACKGROUND

- **Molecular Dynamics (MD)**
  - *MD Simulation*
    - *use computational methods to simulate the movement of molecules in their native environments*



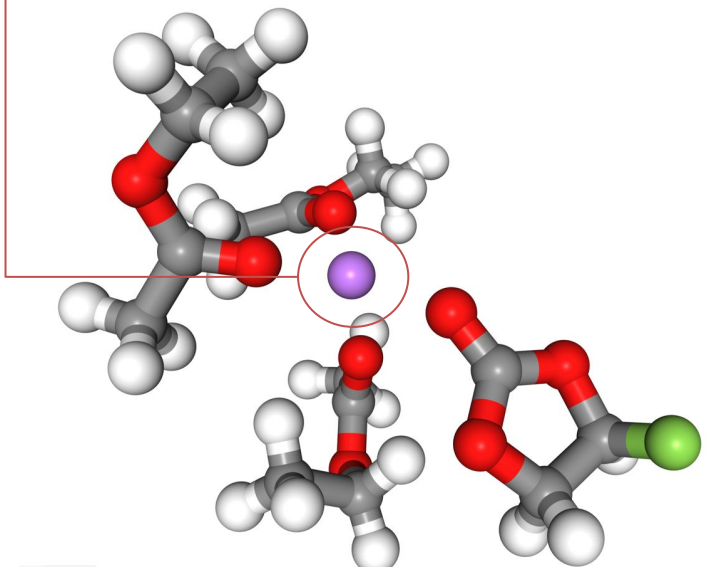
BACKGROUND

- **Molecular Solvation**
  - *Solvation Box*
    - *A solvation box is a computational simulation box that contains a system(solute) surrounded by solvent molecules*



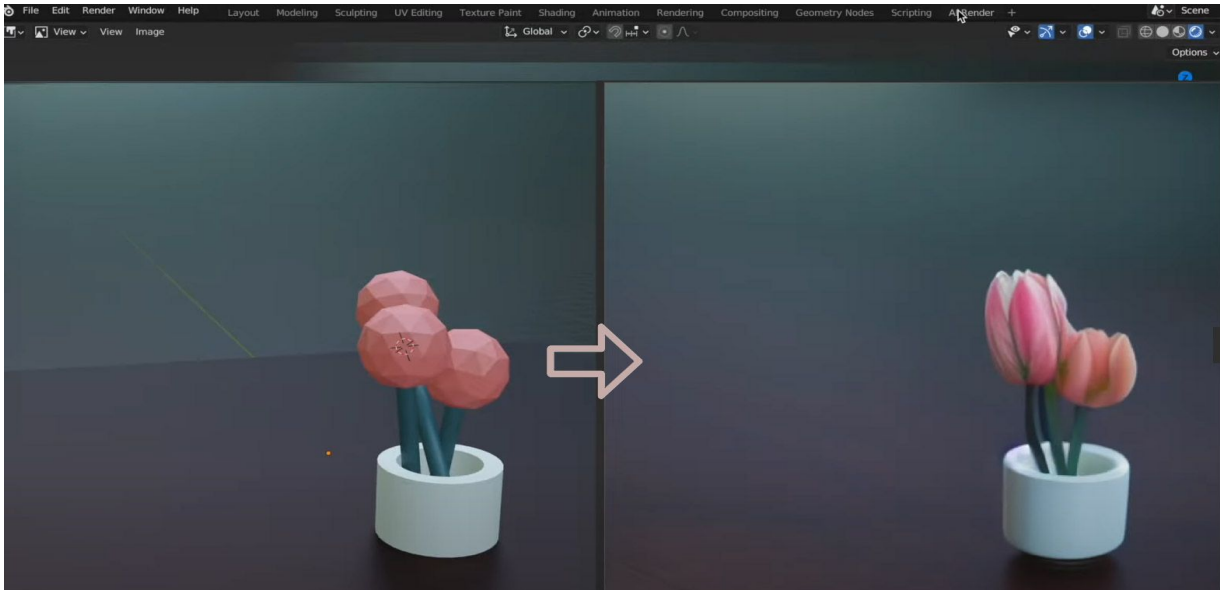
BACKGROUND

- **Molecular Solvation**
  - *Solvation Shell*
    - *Refers to the structured arrangement of solvent molecules that surround a solute*



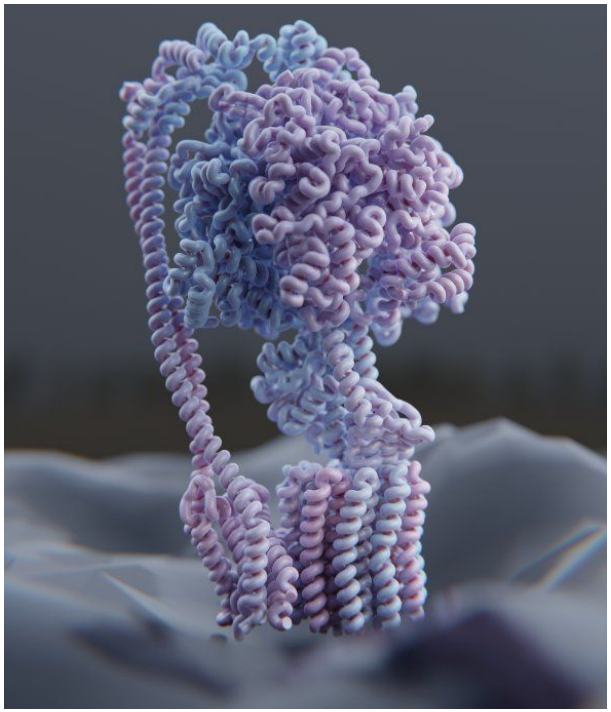
BACKGROUND

- **Software Libraries**
  - *Blender*
    - *open-source rendering software that uses ray-tracing for hyperrealistic visualization*



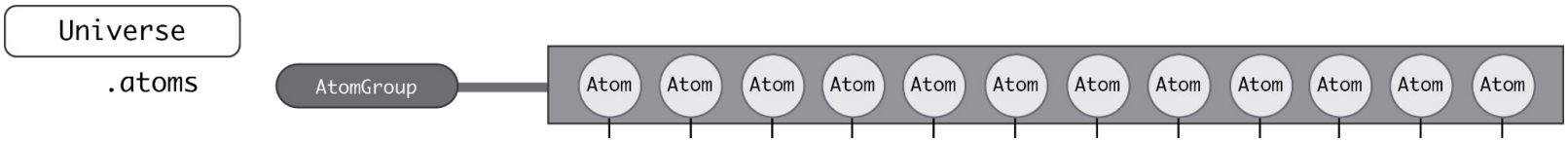
BACKGROUND

- **Software Libraries**
  - *MolecularNodes*
    - *an open-source plugin for Blender, which is a molecular visualization software*



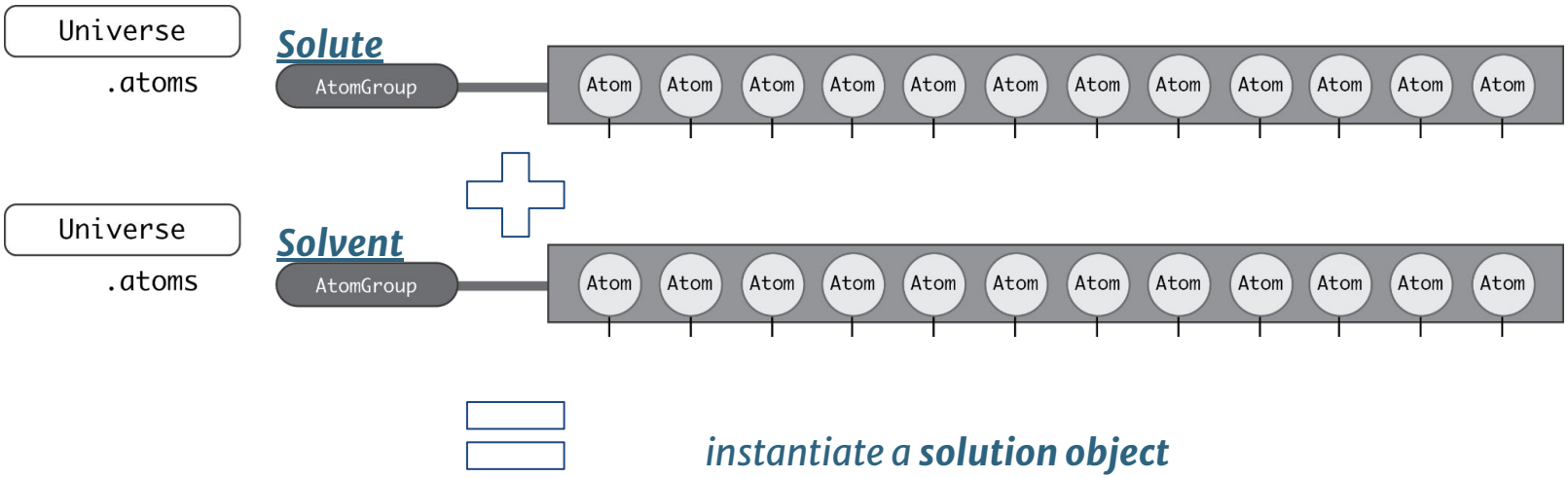
BACKGROUND

- **Software Libraries**
  - *MDAnalysis*
    - open-source software library that reads MD Simulation Data to a data structure (i.e. *AtomGroup*)



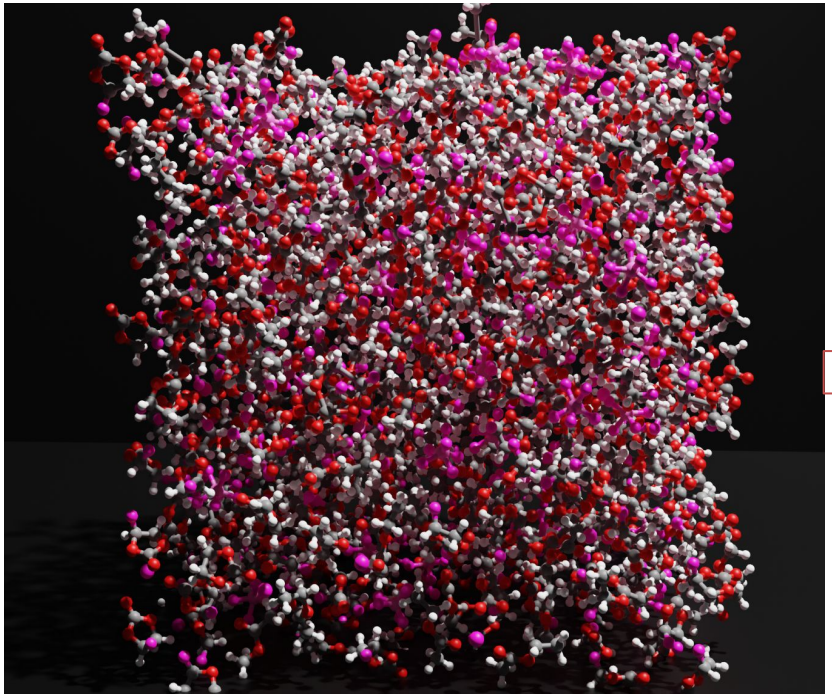
BACKGROUND

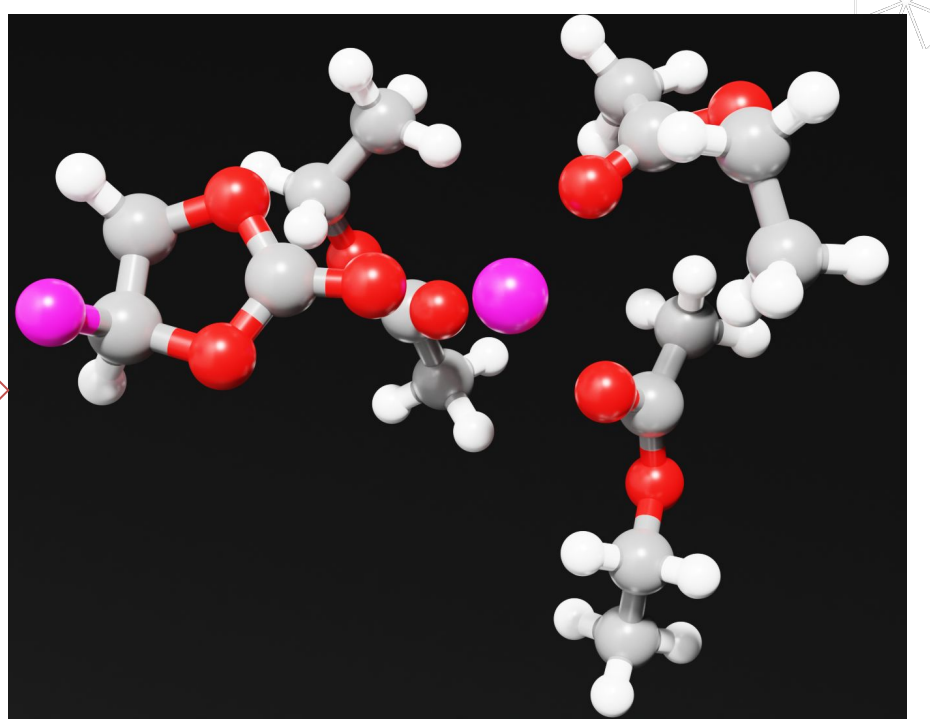
- **Software Libraries**
  - *SolvationAnalysis*
    - open-source software library that extends functionality of MDAnalysis to create a solution object



AIM

- **interoperability** between **MolecularNodes** and **SolvationAnalysis**





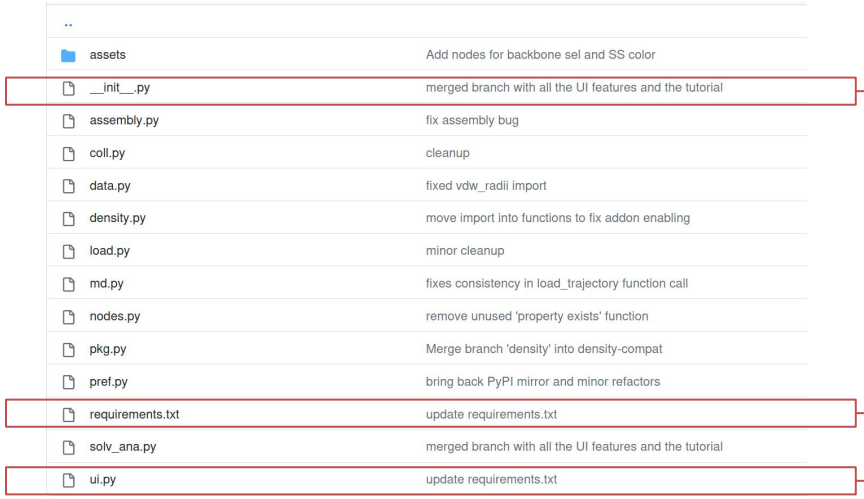
APPROACH

- **Build a Separate Python Module**

..	
assets	Add nodes for backbone sel and SS color
__init__.py	merged branch with all the UI features and the tutorial
assembly.py	fix assembly bug
coll.py	cleanup
data.py	fixed vdw_radii import
density.py	move import into functions to fix addon enabling
load.py	minor cleanup
md.py	fixes consistency in load_trajectory function call
nodes.py	remove unused 'property exists' function
pkg.py	Merge branch 'density' into density-compat
pref.py	bring back PyPI mirror and minor refactors
requirements.txt	update requirements.txt
solv_ana.py	merged branch with all the UI features and the tutorial
ui.py	update requirements.txt

APPROACH

- **Integrate New Module**



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Register all of the properties with Blender to be accessed and modified

Package dependencies

User-interface functionalities

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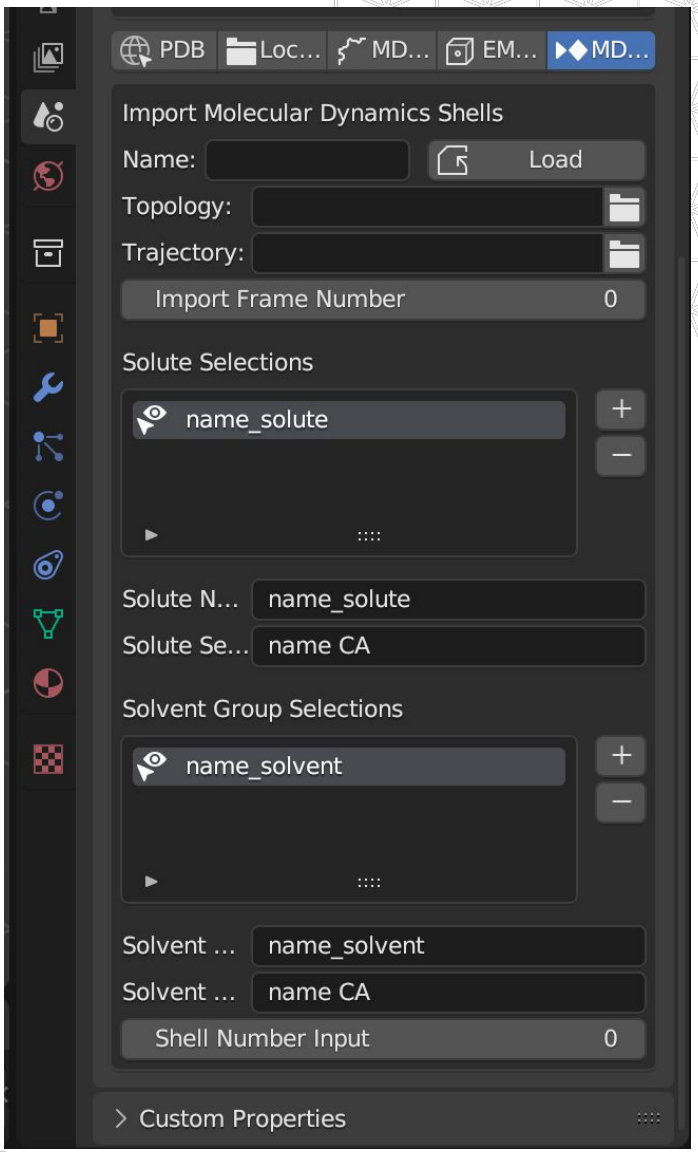
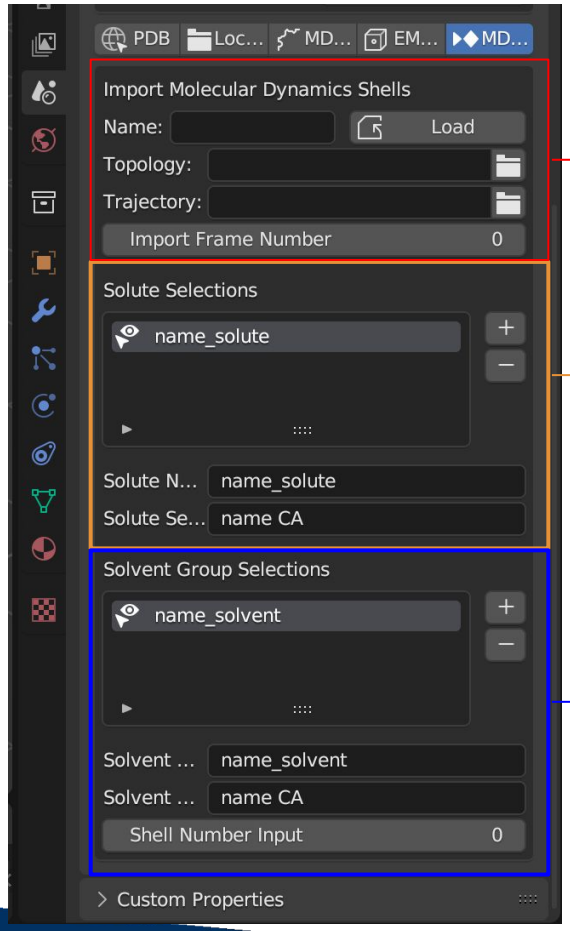
Solvation Analysis User-Interface

- UI to input a selection information



Solvation Analysis User-Interface



Molecular Dynamics Simulation Info

Sets the Blender display name, topology file, trajectory file, and frame of interest.

Solute Selection

Sets the solute of interest using MD Analysis selection syntax.

Solvent Selection

Set parts of the solvent using MD Analysis selection syntax. Specify type of shell to analyze by putting the appropriate number in "Shell Number Input"

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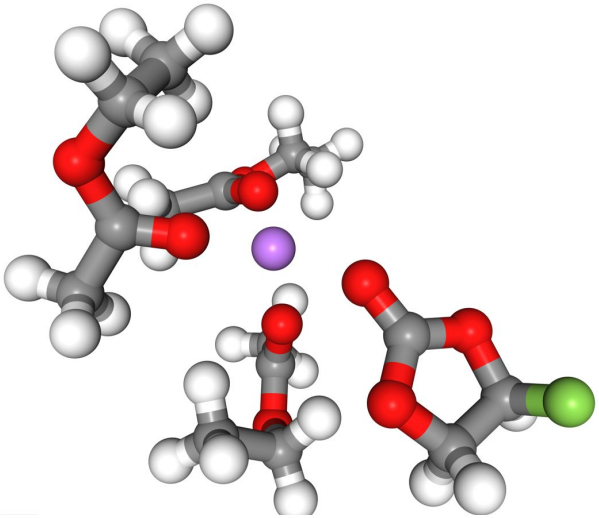
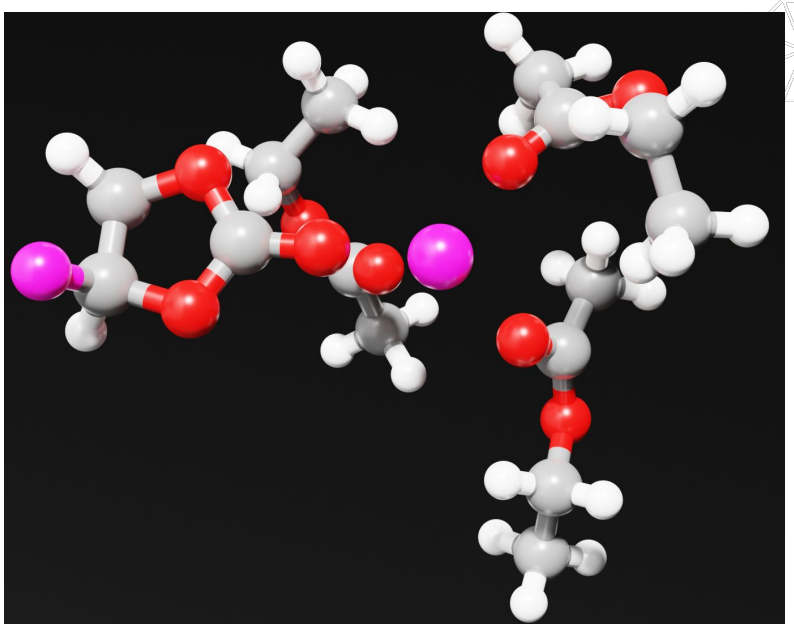
COMPARISONS



NGLView Generated Image



Blender Generated Image

CAPSTONE PROJECT SOFTWARE AVAILABILITY

- Public repository under MolecularNodes in the future it will be available as part of MolecularNodes software distribution

DEMO

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Q&A

Questions?

ACKNOWLEDGMENT

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