
PolyParGen Manual

Release 1

PolyParGen-team

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PolyParGen provides OPLS-AA and Amber force field parameters for polymers or large molecules. In the case that PolyParGen generates OPLS-AA parameters, PolyParGen leverages LigParGen [2] and BOSS [3]. On the other hand, PolyParGen leverages Antechamber [4] and ACPYPE [5] to make Amber parameters. If users want to use the atomic charge of ab initio calculation, user just select the option of ab initio calculation. Ab initio software is NWChem [6].

This site shows how to use the PolyParGen.

Chapter 1

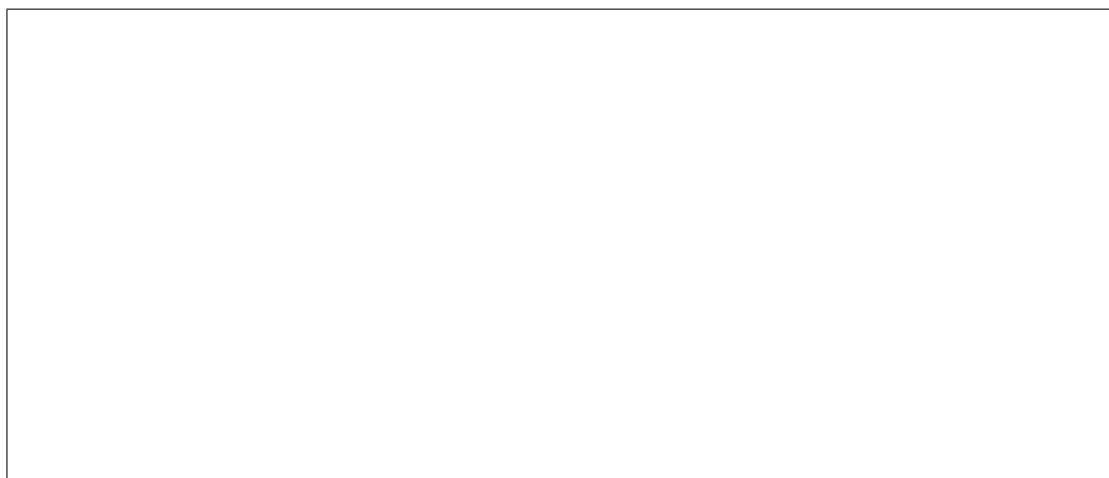
Content

1.1 Usage

In the following it is shown how to use PolyParGen.

1.1.1 Make Molecular Parameter

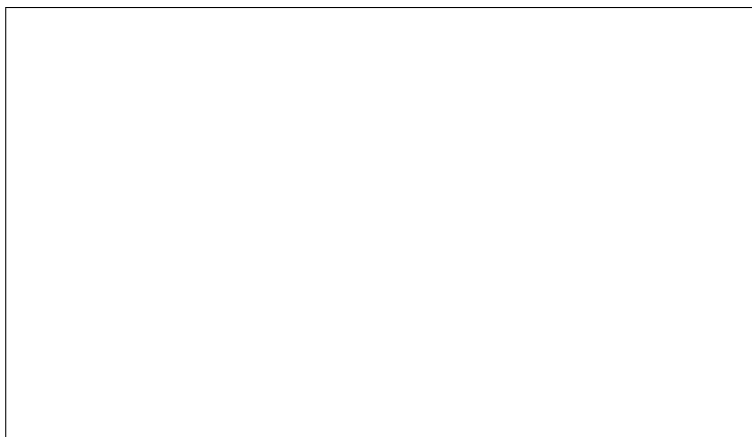
In PolyParGen, Molecular parameters are generated by 2 methods. One of methods is uploading of molecular file. Another method is drawing a molecule. Users can select the method from them in PolyParGen front page.



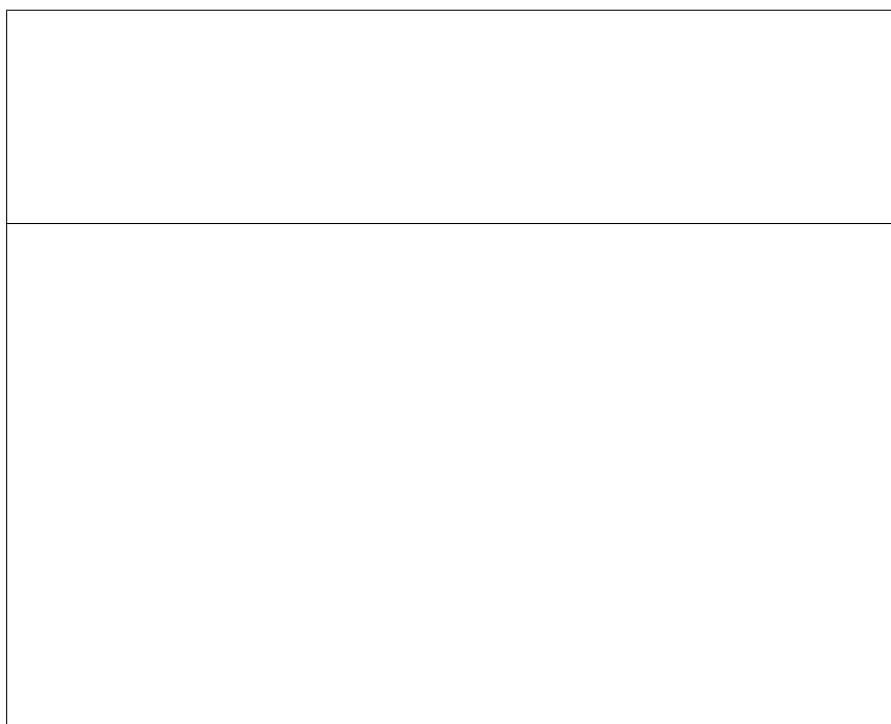
Upload File

This page shows how to make molecular parameter from file uploading.

In the case that users want to make the molecular parameter from their own file, Users push the following image in PolyParGen front page.



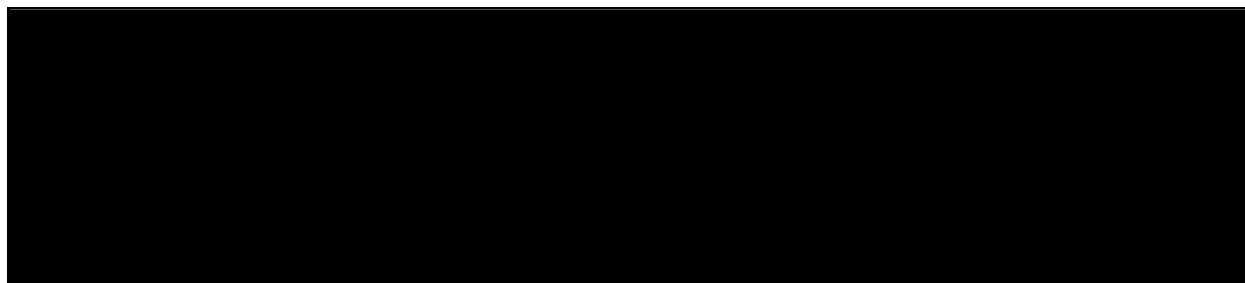
Step1, users have to registrate their information to use PolyParGen. E-mail address certainly is needed in user's information, because PolyParGen sends that parameter file to user's e-mail after generation of molecular parameter. The users, which already registrated, pass this step.



Step2, users upload the molecule file from the following button.

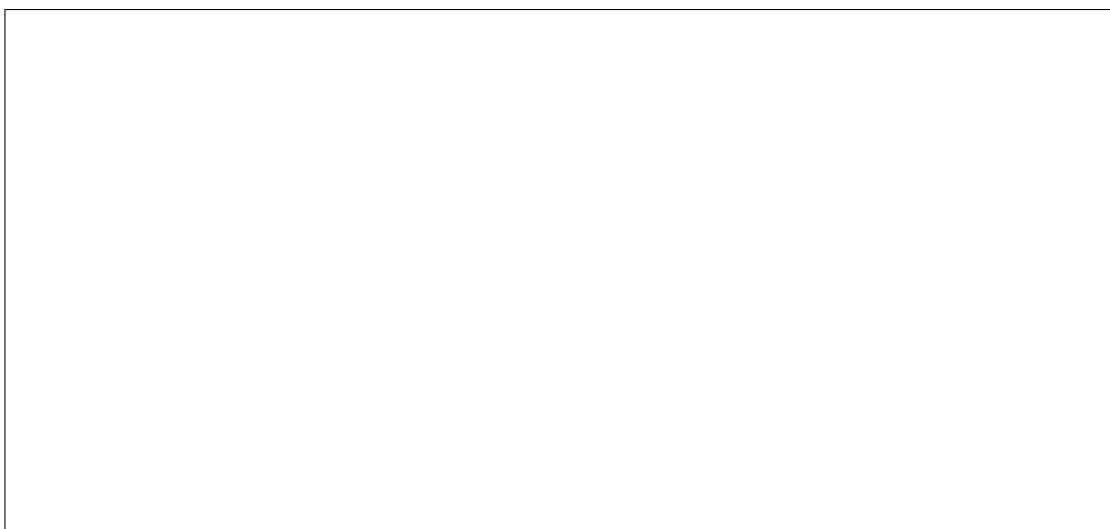


Note: The uploaded file format, which we recommend, is CML file format , because CML file format has more detail for each bond information. CML file can be generated by Avogadro or Open Babel .



Step3, user select the options for making molecular parameter.

This is the window of Step4.



- Select PolyParGen version

At present, the support of PolyParGen version 1 has been suspended to create accurate potential parameters. Users select PolyParGen version 2 (v2).



- Select the type of Lennard-Jones potential

Users select OPLS-AA or Amber parameter. In the case of Amber parameter, users select an atomic charge evaluation method (bcc or gas).

- Set the number of fragment's atoms

Users set the number of atoms contained in one fragment. The default value is 150 atoms. Basically, the default value is recommended.

- Extra options

For large-scale conjugated molecules such as graphene and fullerene, users have to set '0'.

- Whether to evaluate atomic charges by ab initio calculation.

If users want to select the estimated atomic charge by ab initio calculation, users select this option. Also, users have to select the method, basis function and charge density of method. ESP is the electrostatic potential fitting method. Mulliken is Mulliken density analysis.

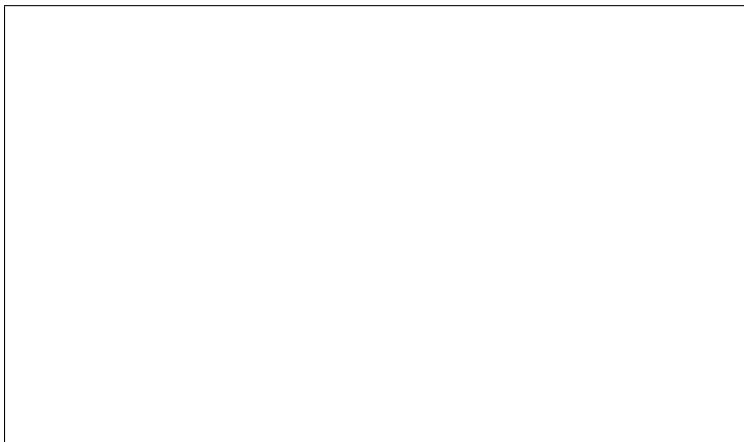
Step4, Input the registered e-mail address. After PolyParGen makes the molecular parameter, the molecular parameter files are sent to the registered e-mail address. Users have to input your e-mail.

Finally, users push 'Submit Molecular' button.

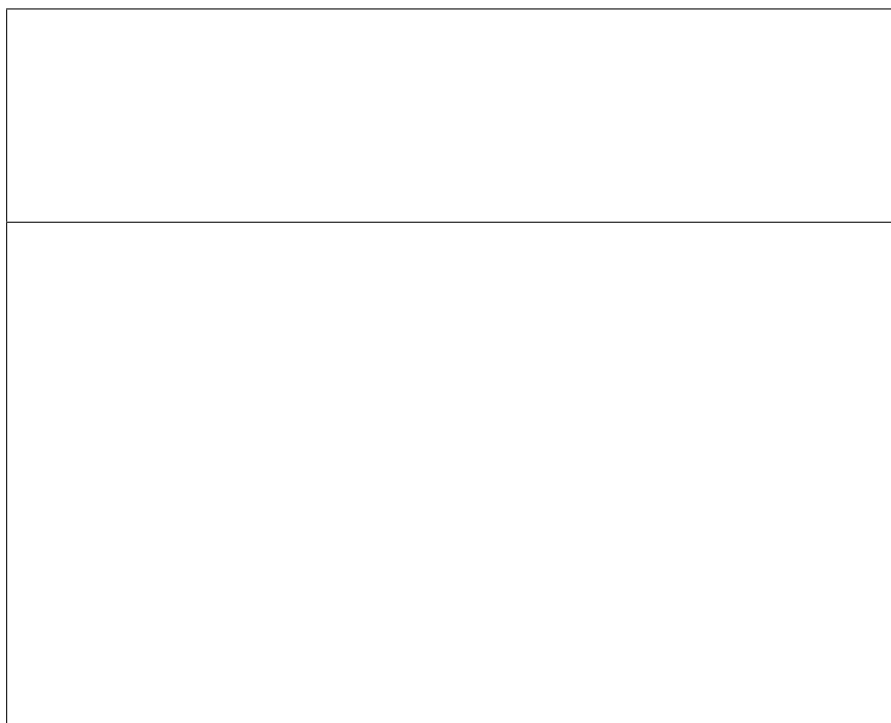
Draw Molecule

This page shows how to make molecular parameter from the drawn molecule.

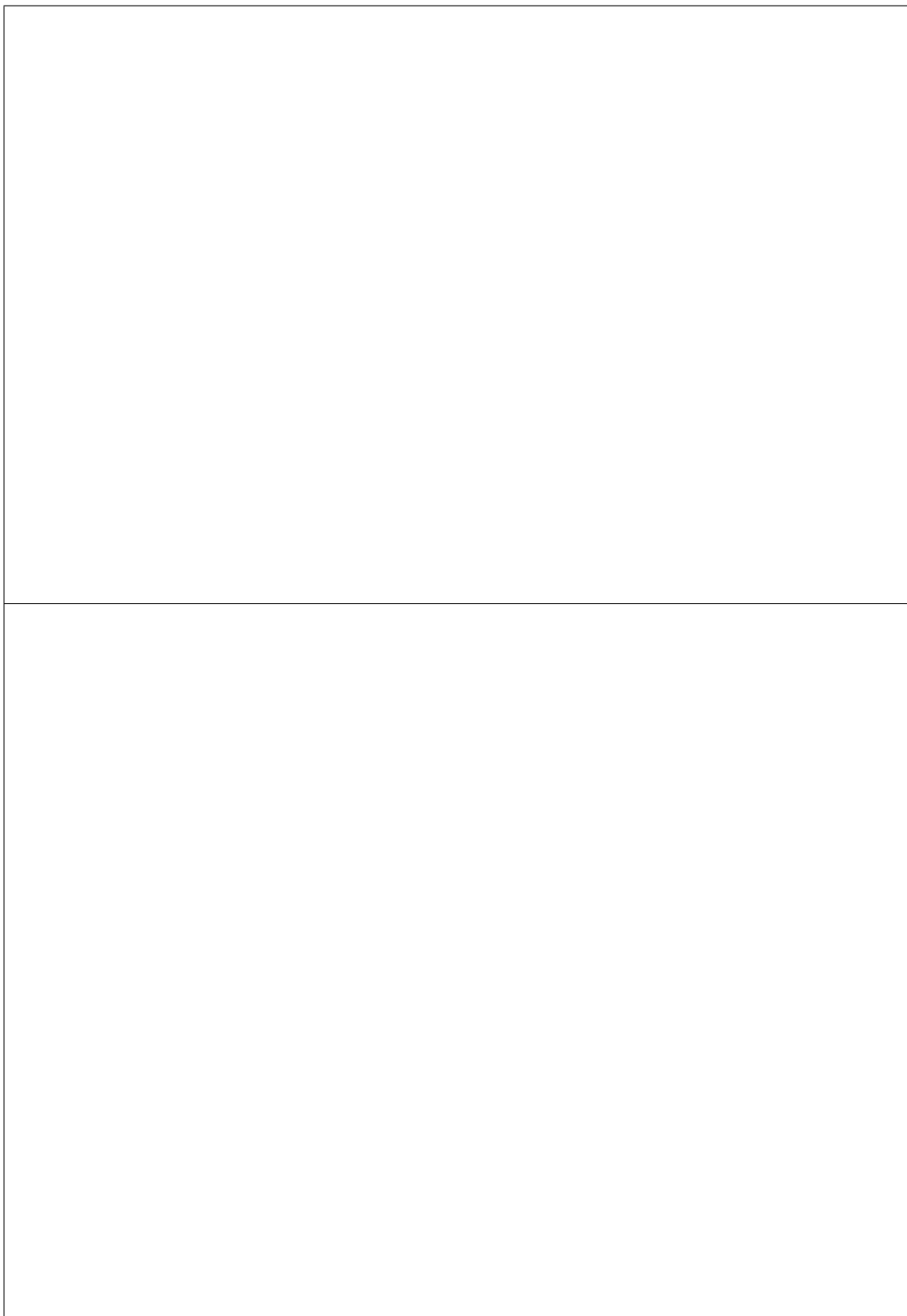
In the case that users want to make their drawn molecules, Users push the following image in PolyParGen front page.



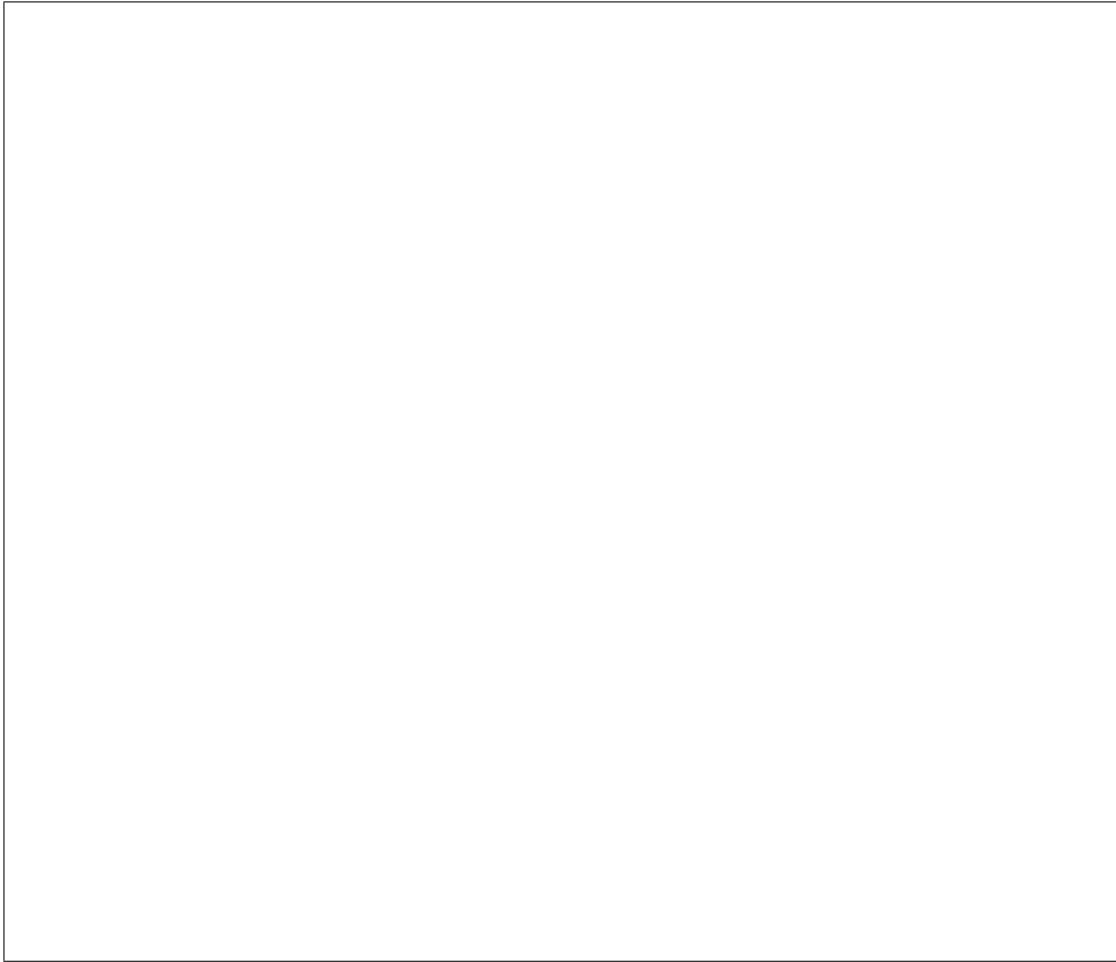
Step1, users have to registrate their information to use PolyParGen. E-mail address certainly is needed in user's information, because PolyParGen sends that parameter file to user's e-mail after generation of molecular parameter. The users, which already registrated, pass this step.



Step2, users draw a molecule under our drawer tool.

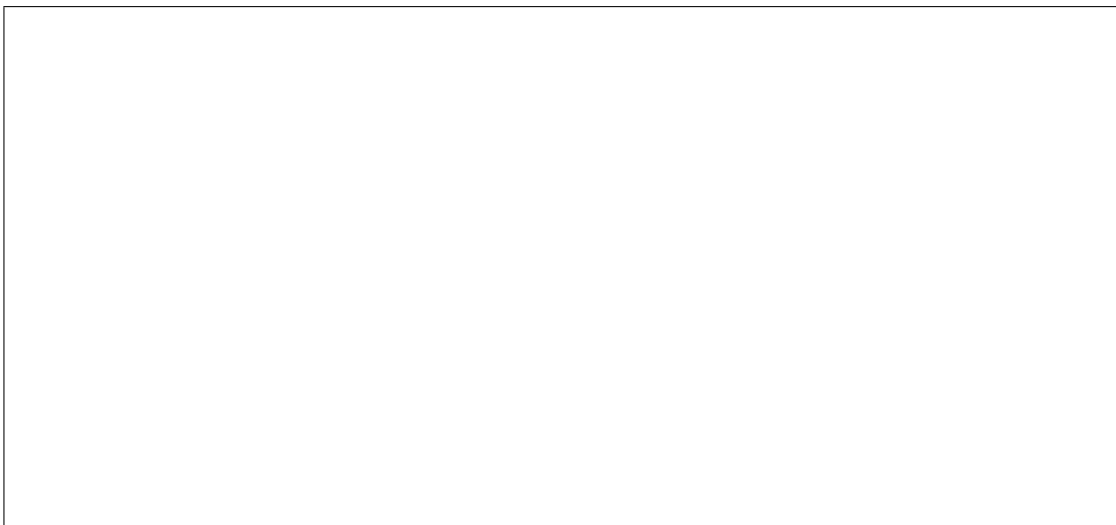


Step3, users confirm the drawn molecule in a 3D structure from with "generate 3D" button. If the molecule has a different structure, users draw the molecule again.



Step4, user select the options for making molecular parameter.

This is the window of Step4.



- Select PolyParGen version

At present, the support of PolyParGen version 1 has been suspended to create accurate potential parameters. Users select PolyParGen version 2 (v2).



- Select the type of Lennard-Jones potential

Users select OPLS-AA or Amber parameter. In the case of Amber parameter, users select an atomic charge evaluation method (bcc or gas).



- Set the number of fragment's atoms

Users set the number of atoms contained in one fragment. The default value is 150 atoms. Basically, the default value is recommended.



- Extra options

For large-scale conjugated molecules such as graphene and fullerene, users have to set "IJ".



- Whether to evaluate atomic charges by ab initio calculation.

If users want to select the estimated atomic charge by ab initio calculation, users select this option. Also, users have to select the method, basis function and charge density of method. ESP is the electrostatic potential fitting method. Mulliken is Mulliken density analysis.

An empty rectangular box with a thin black border, likely representing a missing image or a placeholder for a screenshot.

Step5, Input the registered e-mail address. After PolyParGen makes the molecular parameter, the molecule's parameter files are sent to the registered e-mail address. Users have to input your e-mail.

An empty rectangular box with a thin black border, likely representing a missing image or a placeholder for a screenshot.

Finally, users push "Submit Molecule" button.

1.1.2 Make Molecule

This page shows How to make molecules.

Chapter 2

References

- [1] M. Yabe, K. Mori, K. Ueda, M. Takeda, *J. Comput. Chem. Jpn. Int. Ed.* 5, 2018-0034 (2019)
- [2] Dodda, L. S.; Cabeza de Vaca, I.; Tirado-Rives, J.; Jorgensen, W. L. *Nucleic Acids Research*, Volume 45, Issue W1, 3 July 2017, Pages W331-W336
- [3] Jorgensen, W. L.; Tirado-Rives, J. *J. Comput. Chem.* 2005, 26, 1689-1700. doi:10.1002/jcc.20297
- [4] Wang J, Wang W, Kollman PA, Case DA, *Journal of Molecular Graphics and Modelling* 25 (2):247-260 (2006)
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- [6] M. Valiev, E.J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, W.A. de Jong, *Comput. Phys. Commun.* 181, 1477 (2010)