Development of OpenMX Viewer

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http://www.openmx-square.org/viewer

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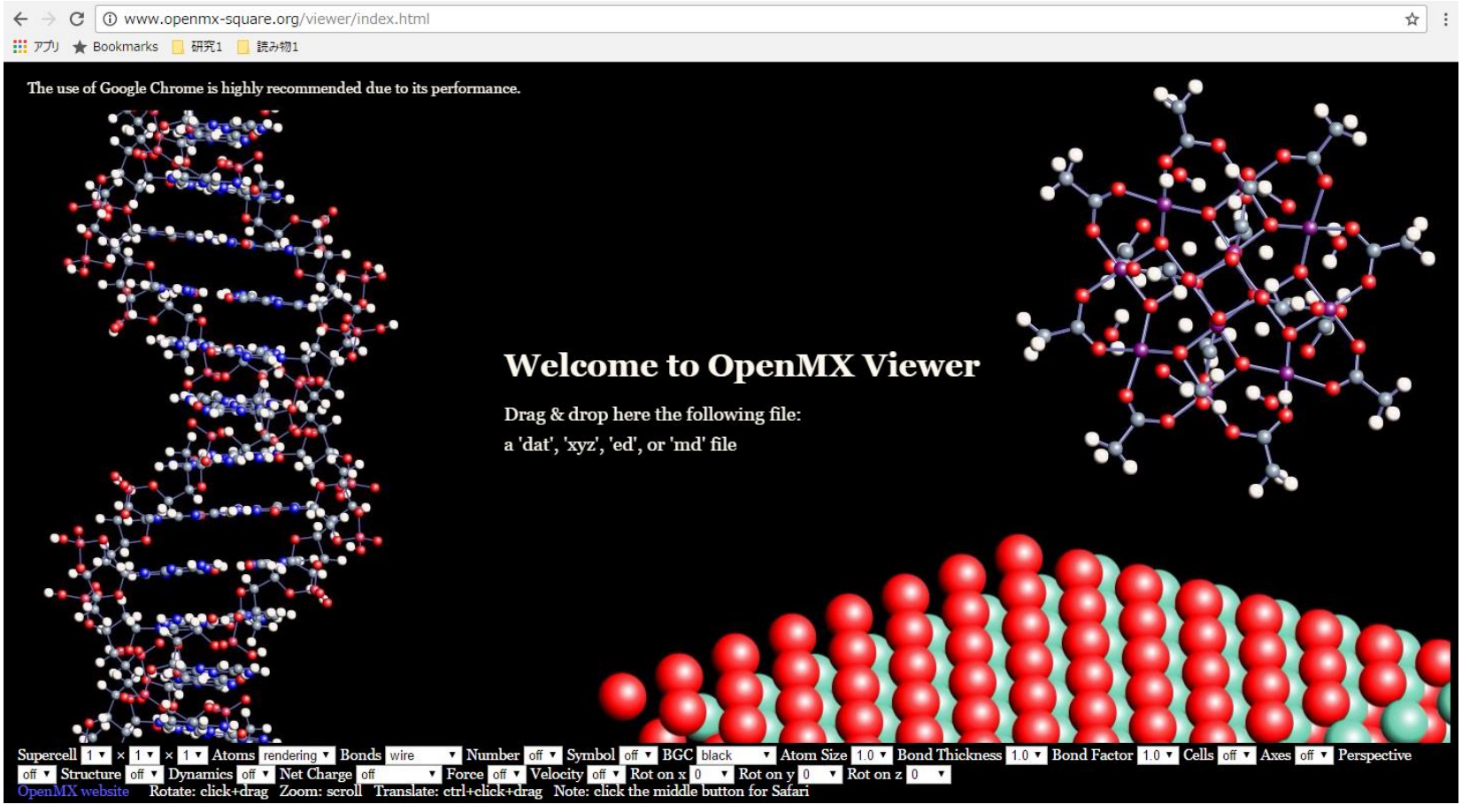
Release of OpenMX Viewer

We have released the OpenMX Viewer on Aug. 19th, 2016.

- GNU-GPL v3
- User friendly interface: drag and drop
- Analysis of structure, geometry optimization, and charge



WEB-based GUI

- WEB browser is one of the most familiar interface that people spend a long time.
- Any machine dependent problems such as OS and version can be absorbed by WEB browsers in principle, which results in that a single frame will work for many different platforms like Windows, Mac, and Linux.
- No downloading and no plugging-in and no updating are required for users.
- Developers only have to change and modify codes on the server, by which all the users can get benefit.
- Many tools have been developed so that WEB-based GUI is fast and easy to use.

Tools for WEB-based GUI

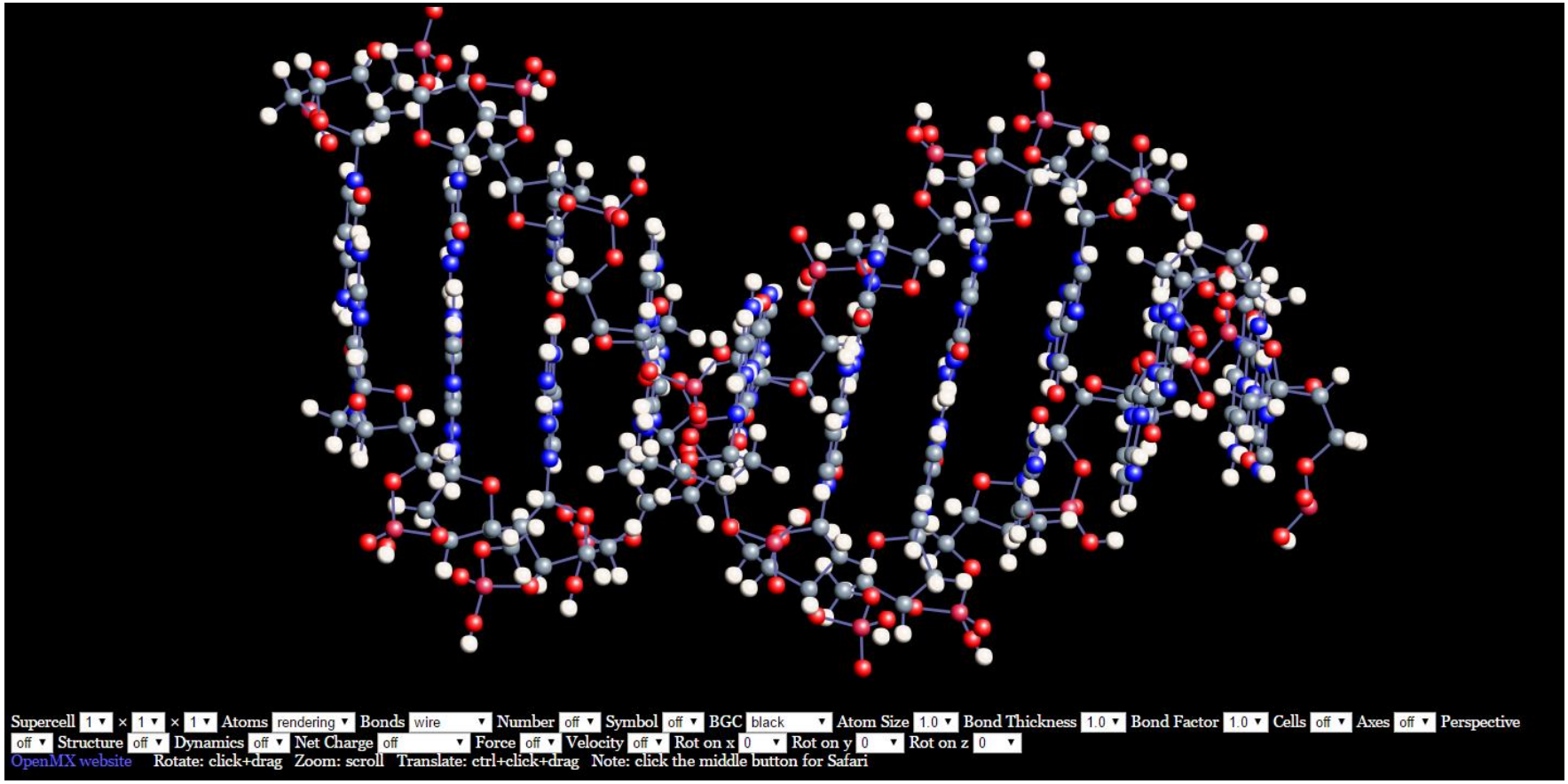
- HTML5
- CSS3
- Javascript
- Canvas2D
- WebGL
- CGI

Current status of OpenMX Viewer

- 6611 lines written by html5, css3, js, and canvas2d
- dat, xyz, and md files are readable
- Rotation, zoom, and translation
- Easy change of atom size, bond thickness, and bond factor
- Atom index and atom symbol
- Supercell representation
- Structure analysis
- Analysis of geometry optimization
- Charge analysis
- Google Chrome recommended due to its performance

Easy check of a dat file

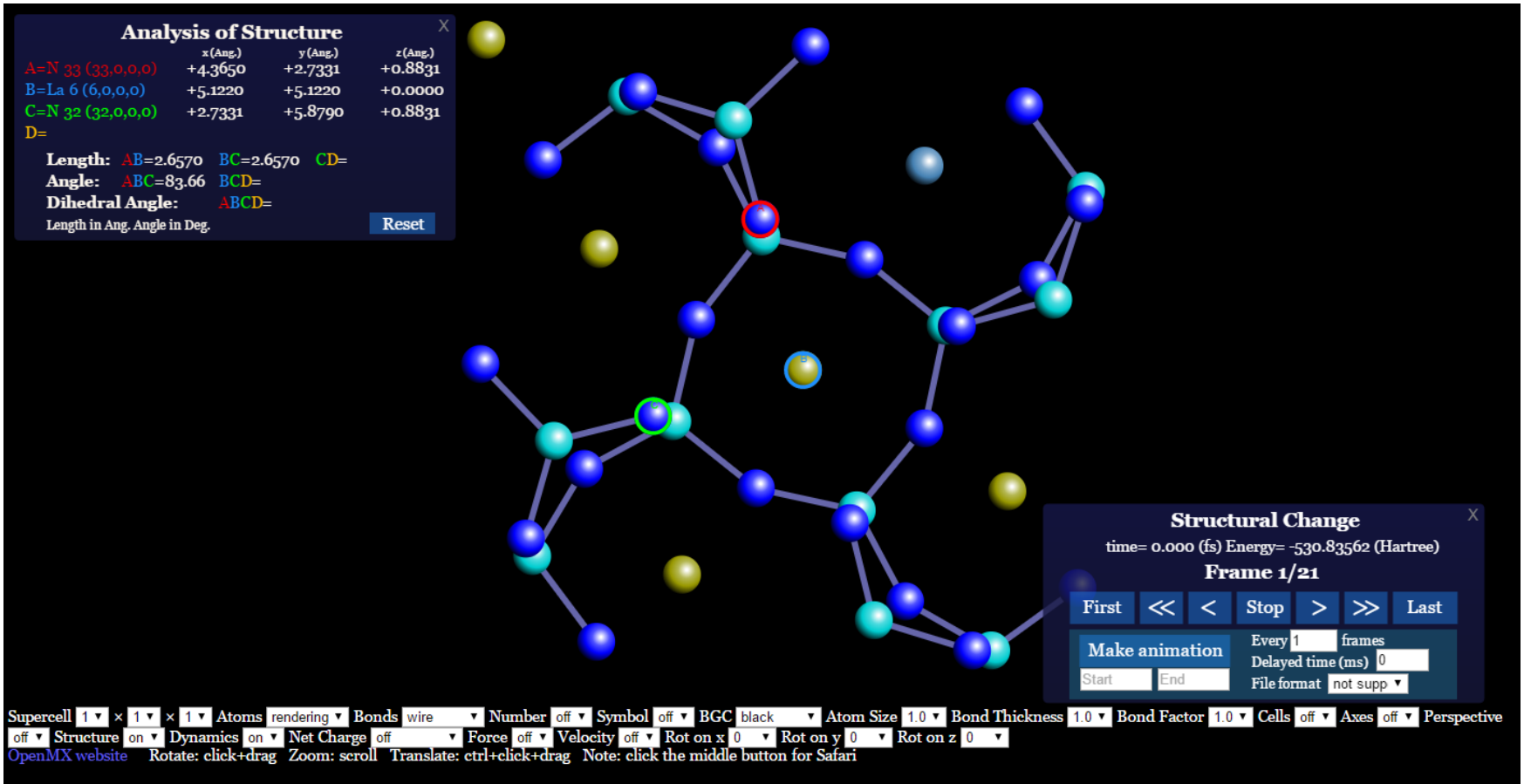
A dat file can be easily checked by drag and drop to any browser.



Analysis of structure optimization

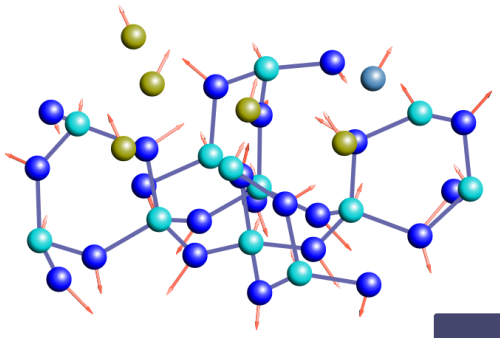
A md file can be easily analyzed by drag and drop to any browser.

- Trace of optimization process
- Analysis of structure
- Check residual forces

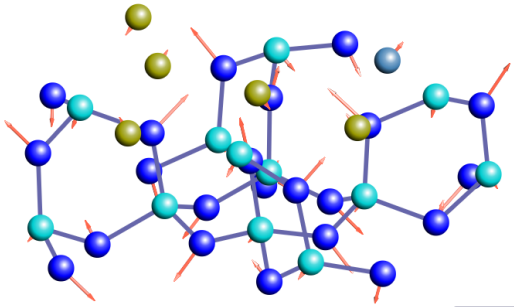


Analysis of structure optimization

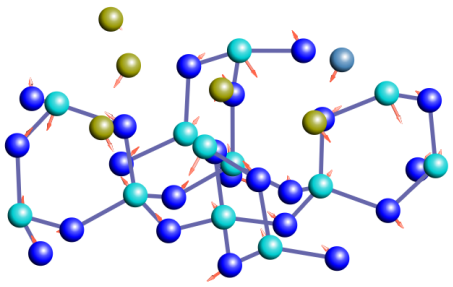
Residual forces can be visualized by vectors.



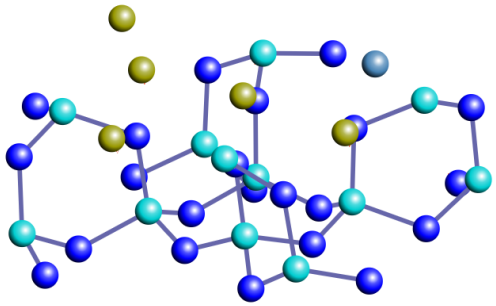
1 step



10 step



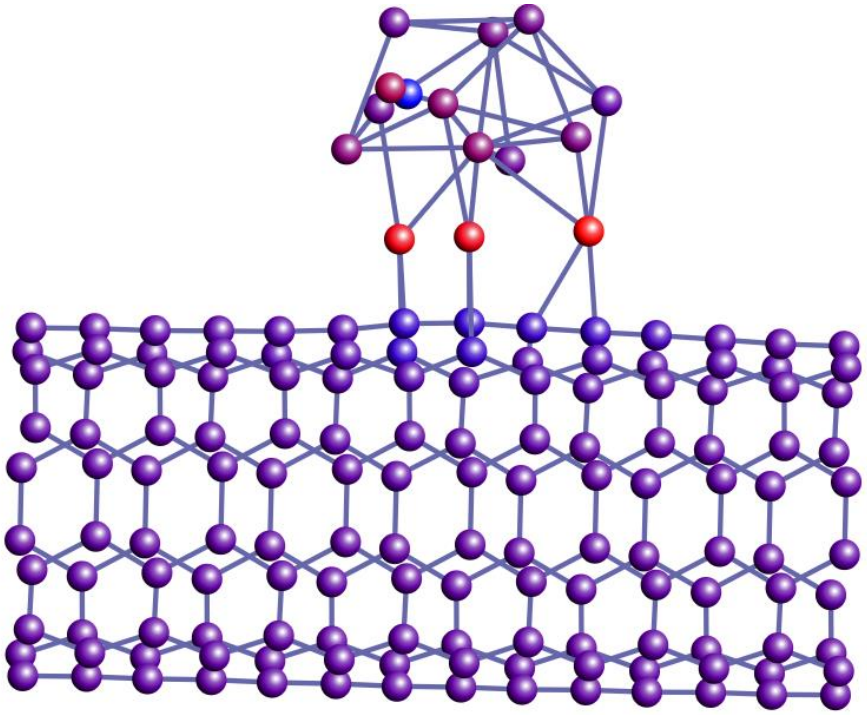
14 step

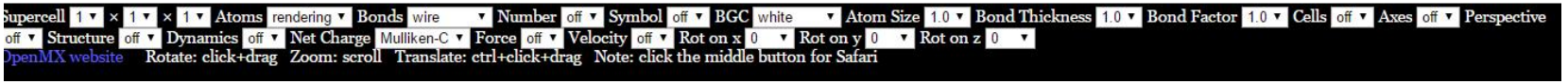


21 step

Analysis of structure optimization

Using a md file, one check easily check spatial charge distribution.





Summary

- OpenMX Viewer is a web-based GUI.
- The web-based GUI enables us to quickly visualize crystal and molecular structures in input and output files of OpenMX by simply drag and drop, and analyze structural parameters such as bond length and bond angle in a convenient way. Several basic functionalities such as analysis of Mulliken charges, molecular dynamics, and geometry optimization are also available.
- We will soon support cif files, and a functionality which generates a template of an input file with the provided geometrical structure for OpenMX.
- It is also interesting to develop a cloud system with the OpenMX Viewer.