Web-application for computational materials design

Project goal and target auditory

In this project, you shall create a web-application for computational materials design, which relies on original scientific insights and verified computational routines.

The web-application will be used by a world-wide community of scientists and engineers interested in novel type electrolytes known as ionic liquids.

Background

High-throughput computational materials design is an emerging area of materials science. This new approach to materials design allows even non-scientists to generate, manage and analyze enormous data repositories. For example, play with build-a-battery.meteor.com.

Architecture and programming

The web-application should do the following simple steps: (1) allow user to read/write files on the server via a web interface; (2) execute scripts on server; (3) show/plot the data responded by the server in the web-interface.

With the full support from the group lead by the client, you are expected (1) write a simple web-interface for desktop using HTML5/JS; (2) write server side code to enable read/write/execute functional; (3) implement simple plotting functional using HTML5/JS.

The last step should result in a webpage similar to the presented on the right – here variation of chemical structure (TOP) will be visually reflected in change of electrochemical and physical properties (MIDDLE and BOTTOM). The data for showing and plotting will be generated by the server scripts which will be provided by the client.

Prerequisites or willingness to learn:

- Knowledge of HTML5 and JS;
- Basic knowledge of a server-side language, like PHP or python;
- Elemental knowledge of bash and Linux servers.
Licensing

The whole project will be open source. It would be nice to keep the development using a repository hosted on git-hub.

About the client

Hi, I am Vladislav Ivaništšev from the University of Tartu. My current research focuses on the electrochemistry of ionic liquids and employs computer modeling. Importantly, I have very good experience of using all the software required in this project and have good skills in HTML5/JS. Moreover, I have already supervised two Software projects in 2010, and will support you in this project.

More info: linkedin.com/pub/vladislav-ivanistsev/40/479/1a7, and researchgate.net/profile/Vladislav_Ivanistsev and github.com/olunet

Opportunities

If only you wish so, this project gives several opportunities to practice in setting Linux server via Docker technology in clouds, or running Quantum Chemical calculations to generate data for plotting, or using advanced features of HTML5. Besides the main tasks (in overtime) you are very welcome to try any relevant activity (for fun and learning) and will be supported in it by the client.