

2022-09-29 FF optimization for MD simulations binder-inorganic surfaces

Date

29 Sept 2022

Attendees

- [Sikora, Ben](#)
- [Stefan Knippenberg](#)
- [Ma, Changru](#)
- [Guillaume, Maxime](#)

Aim of meeting

The Utility of Dongyue Liang (UChicago, group of Juan de Pablo) to generate a FF for these interfaces has to be internalized. The utility has been developed in the framework of a collaboration on conductivity on interfaces between the UChicago group and the group of Prof. Marzari at EPFL.

Maxime stresses the transversal character of the task – this activity has to be done in a Sim&Mod framework. Ben got the source code from Phillip Rauscher, who left for Paternity leave. The code has been put on the Solvay_rni Gitlab directory. Attention has to be paid to the Confidentiality restrictions: results of the EPFL/UChicago work cannot be shared over the Sim&Mod network.

General Notes

1. Internalize. Ben knows that the code is not user friendly nor adapted to be used on different materials. Scripts have to be written to avoid hard-coded choices. Before reshuffling this task back to the UChicago collaborator Dongyue, who is paid by Solvay, Ben would like to investigate the code and evaluate whether he can do these adaptations himself.
2. Definition of three example-targets (one for Mat GBU, one for Battery, one for Novecare)
An extra problem is that nor Changru nor Stefan has access rights on the Gitlab. Ben works out an hierarchy with branches and secured repositories. The code will be placed on a general Sim&Mod repository – as such, the Novecare and Battery workers do not see the work of the Materials GBU.

All information concerning these activities (except for the code itself, which is put on the Gitlab) can be put on the shared drive

<https://drive.google.com/drive/u/0/folders/1SnI4gfUIC7QQzHh-Ap1kShnlfMIYbWe>

Information on Gitlab and best practices can be found on [GitLab Best Practices](#)

Action items

- ✓ Sikora, Ben Evaluate code for adaptation of generalized input files. 20 Oct 2022
- ✓ Sikora, Ben Submission of Sim/Mod Network GitLab repository to IT05 Oct 2022
- ✓ Sikora, Ben Mirror repository Polymer Physics Sim/Mod network 20 Oct 2022
- ✓ Sikora, Ben Begin to formulate structure around best practices for GitLab 20 Oct 2022
- ✓ Sikora, Ben Set up meetings for best practices of GitLab and to review code 30 Sept 2022