

Comments to database functionality

1. Validated records are always available in the view mode. Login is needed to validate records (to be done by ORSO members)
2. Inputs are not case-sensitive
3. Parameters like temperature can be entered. If not available not presented on the page
4. Units for all entries should be added.
5. It is possible to enter same compound with e.g. different temperature
6. SLD value is available from main table if entered manually
7. For more complex systems e.g. Lysozyme with 40% D2O, ISIS calculated for proteins may be linked <http://psldc.isis.rl.ac.uk/Psldc/>. The calculator has some limitations, a) not suitable for X-rays(?) b) Volume is calculated from amino acid sequence.
8. Distinction between calculated and experimentally determined parameters
9. It should be possible enter material with email (optional) for future reference and validation process. Email won't appear in API record. And it should be clear what are terms of using the email
10. It needs to be established Who has authority to validate/invalidate entries? And How to filter invalid entries
11. Once functionality is sorted out Instructions will be provided
12. Python API may be available from pip
13. Scattering length can be provided separately to SLD (per element), so one can do calculation on their own
14. How to include energy dependent slds? Christy thinks is good idea to include. Latest version of periodictable may have some of these.
15. Magnetic SLD is provided. Christy's provided additional spreadsheet to be added to database.
16. Refractive indexes – to be established if this useful entry
17. Input from MD simulations column can be added.
18. Magnetic field column to be added
19. Pressure (surface) can be added in comment field
20. Absorption calculations may be useful
21. We need to define, which of the entry fields are required.
22. How to extract entry for particular physical states – search will be added in the future (advance mode).
- 23.
24. Units: the same in the attached spreadsheet from Christy.
 - a. Molar Volume (cm³)
 - b. Number Density (N) in Atoms/Angstrom³
 - c. Temperature in K but C may be needed
 - d. Formula Volume Å³ and nm³
 - e. Energy currently in eV to be checked if possible in keV
25. SLDDDB currently hosted at ESS but it may be renamed. Suggestion: slddb.reflectometry.org
26. Tags: What is difference between polymer and synthetic polymer?

Next steps

- Volunteers for testing: Jos, Alessandra, Alex, Tom and Bridget

- Artur happy to continue developing
- ESS will continue hosting server. Wojtek in charge and will help Artur debugging