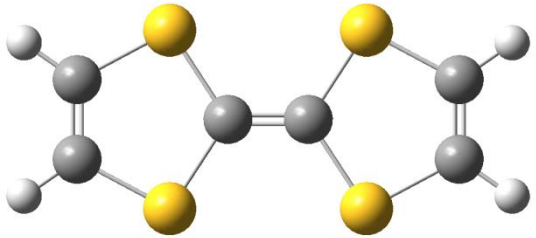
Dr. Artem V. Sergeev
Research scientist at
SkolTech and
Moscow State University

Took CCMM course in **2014:**
1st year PhD student
at MSU, Phys. dept.

Final project:

Investigating the capability of the redox-potential computational studies

Tetrathiafulvalene (TTF) redox-mediator



TTF/TTF^{+} and TTF^{+}/TTF^{2+} potentials were calculated using different functionals, basis sets and implicit solvation models (IEF, CPCM, SMD).

- Gas phase calculations are absolutely not reliable for description of charged species in solution (potential error up to several V).
- All considered solvation models result in a considerable error about 0.5 V for both TTF/TTF^{+} and TTF^{+}/TTF^{2+} potentials.
- Explicit consideration of 1st solvation shell is crucial for accurate simulation of redox reactions