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## Web-based service to generate molecular topologies

Molecular simulation is a powerful tool to derive properties of molecules and materials. The technique is based on numerical simulation solving Newton's equation of motion ( $F = m a$ ) for many atoms, where the forces are derived from an analytical energy function  $V(r_1, r_2, \dots, r_N)$  by  $F_i = -dV/dr_i$ . One of the main issues preventing widespread use of molecular simulation for arbitrary materials is the energy function.

Our lab has developed a C++ toolkit, Alexandria, to derive parameters for molecular mechanics force fields from experimental data and quantum mechanics calculations. Alexandria also computes atomic partial charges and generates topologies (input files) for organic molecules to be used in molecular dynamics simulations and applications, for instance in drug design.

This master project aims to design a web-based service in order to facilitate the usage of Alexandria force field in large-scale applications such as drug discovery and material sciences. The student will mainly code in Python to develop a GenTop (Generate Topology) web server and will also gain experience working with the GROMACS and OpenBabel software packages.

Requirement for the student working on this master project (30-45 points) is a solid background in computer science, IT, or similar, and in particular good programming skills in Python. Programming skills in C++11, experience with SQL databases and basic knowledge in chemistry and physics are a bonus.

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