Project 6.4. Phase-Amplitude Functional Theory – implementation and development

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Background:
Phase-Amplitude Functional Theory is based on quantum mechanical equations and will allow solving many body problem with less computational effort needed than typical generalized gradient approximation density functional theory GGA DFT. Less computational effort will allow to simulate larger systems i.e. crystal steps or larger area of electronic devices. Computational complexity deterioration results directly from the character of the new equations in which basis functions are used to write solutions for the phase of the wave function and its amplitude. Basis functions may be smaller because the equation's solutions are much less "oscillating" than typical solutions of one-electron wave functions in typical DFT electron density functional theory. The project first implies the implementation of the theory equations. After successful implementation, the next point will be to check whether the method gives good results, i.e. we will compare the simulation results using the PAFT method and the results obtained using DFT implemented in SIESTA and VASP for small molecular systems. After successfully testing the method, we will proceed to simulate and obtain properties of larger systems, i.e. atomic steps or large active area of electronic devices. As a result of project implementation, a method better in terms of computational efforts than DFT will be obtained. We plan to perform numerical calculations using a new PAFT theory as well as with standard DFT software.

Aim:
The scientific goal of the project "Phase-Amplitude Functional Theory – implementation and development" PAFT will be to construct method equations, implement them in a computer program and check the properties obtained for simple molecular systems, as well as predict the properties of optoelectronic devices such as electroluminescence LED diodes, LD laser diodes and electromagnetic radiation detectors.

Requirements:
- DFT simulations, data analysis experience
- Bachelor or Master degree, or relevant working experience
- written and oral communication skills in English
- experience in programming with C/C++ in a Linux environment
- knowledge of a scripting language, one of Python, Perl, bash, cs