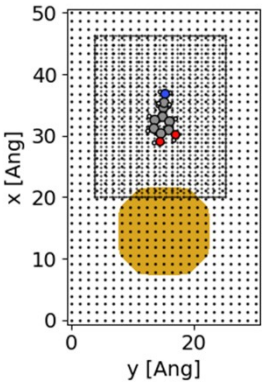
Project Ideas – GSoC 2023

Functional Nanosystems Group, University of Freiburg

I. GPAW Project: Hybrid Quantum/ Classical simulations



Mentor: Michael Walter (GitLab: @mwalter)

Description

How does light interact with plasmonic materials and what are the optical properties of nanoparticle-molecule assemblies? The project task is to extend and improve the current implementation of the hybrid quantum/ classical scheme in GPAW [1] and tackle some of the challenges outlined in the GPAW documentation. The current implementation uses a finite-difference time dependent approach described by Coomar et al. [2] for the classical part of the simulation (i.e., the plasmonic nanoparticle) and the molecular subsystem is modelled using time-propagation density functional theory. The two subsystems are coupled through a common electrostatic potential. This method provides a fast and computationally inexpensive way to calculate the optical spectral of combined nanoparticle-molecule assemblies and the results are shown to have good accuracy, comparable to more computationally expensive all-quantum methods [3].

Expected Outcomes

The contributor will choose one of the following approaches for the new implementation:

A. Write an interface to an external open-source finite-difference time-domain code, such as MEEP;
B. Implement an approach based on the time-domain boundary element method [4], [5];
C. Extend the functionality and improve the performance of the current quasi-static implementation.

Besides the main coding task, the contributor will add relevant benchmark cases/ tests to the code (e.g., compare plasmonic spectra with Mie theory) and update the relevant documentation. At the end of GSoC, the contributor will present their work as a tutorial for the Functional Nanosystems group.

Extension Tasks

- Add the effects of a background medium by using a different normalization for the permittivity of the classical material ($\epsilon_\infty \neq \epsilon_0$)
- Read nanoparticle geometries from 3D model files and improve visualization of input structures

Getting Started

A good place to start is with the GPAW documentation on classical electrodynamics. Below there is also a reading list with several papers about the hybrid quantum/ classical scheme and the implementation in GPAW. The contributor should also be familiar with the workflow for making new contributions to the code (GPAW follows the same workflow as the Atomic Simulation Environment).

Required Skills: Python; effective written and spoken communication skills.

Desirable Skills: Knowledge of plasmonics; experience with density functional theory code or classical electromagnetism simulations.

Size of Project: 350 hours

Difficulty Level: Medium

Reading List

[1] A. Sakko, T. P. Rossi, and R. M. Nieminen, 'Dynamical coupling of plasmons and molecular excitations by hybrid quantum/classical calculations: time-domain approach', *J. Phys. Condens. Matter*, vol. 26, no. 31, p. 315013, Jul. 2014, doi: 10.1088/0953-8984/26/28/315013.

[2] A. Coomar, C. Arntsen, K. A. Lopata, S. Pistinner, and D. Neuhauser, 'Near-field: A finite-difference time-dependent method for simulation of electrodynamics on small scales', *J. Chem. Phys.*, vol. 135, no. 8, p. 084121, Aug. 2011, doi: 10.1063/1.3626549.

[3] J. Fojt, T. P. Rossi, T. J. Antosiewicz, M. Kuisma, and P. Erhart, 'Dipolar coupling of nanoparticle-molecule assemblies: An efficient approach for studying strong coupling', *J. Chem. Phys.*, vol. 154, no. 9, p. 094109, Mar. 2021, doi: 10.1063/5.0037853.

[4] S. Pipolo and S. Corni, 'Real-Time Description of the Electronic Dynamics for a Molecule Close to a Plasmonic Nanoparticle', *J. Phys. Chem. C*, vol. 120, no. 50, pp. 28774–28781, Dec. 2016, doi: 10.1021/acs.jpcc.6b11084.

[5] G. Dall'Osto, G. Gil, S. Pipolo, and S. Corni, 'Real-time dynamics of plasmonic resonances in nanoparticles described by a boundary element method with generic dielectric function', *J. Chem. Phys.*, vol. 153, no. 18, p. 184114, Nov. 2020, doi: 10.1063/5.0022329.