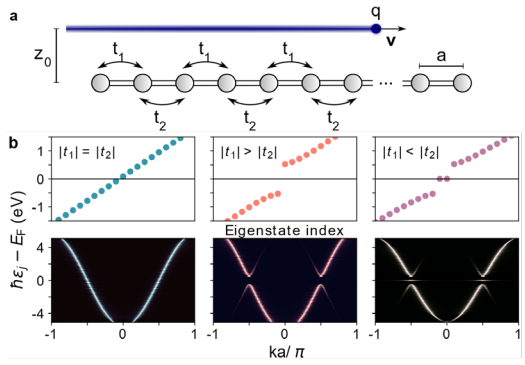
Draft of Bachelor/Master project. For more options, visit polima.org.

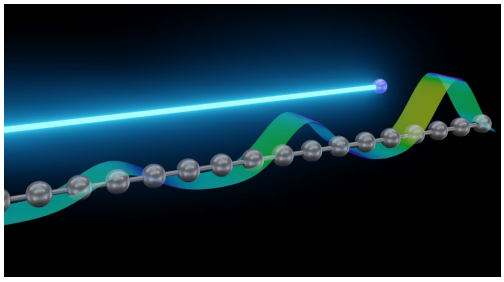
Project title: Improved modelling of optical response using tight-binding chains

Proposed by: Line Jelver	Possible supervisor(s): Line Jelver

PROJECT DESCRIPTION:

Tight-binding models are extremely useful in describing trends in the behavior of solid-state materials. The Su-Schrieffer-Heeger model describes an atomic chain with alternating hopping amplitudes which allows for a tuning of the electronic properties in the chain between a semiconducting and metallic behavior. It was originally introduced to describe polyacetylene using a tight-binding description for the p_z electrons and elastically coupled CH monomers [1,2] but has been applied to simulate a great variety of material properties and how these depend on the electronic structure; Examples are band structure effects on the extreme nonlinear optical response produced by strong laser fields [3,4] and on the nonlinear effects in the cathodoluminescence produced when a slow electron travels by the chain.[5]





The aim of this project is to utilize the SSH model to investigate trends in light-matter interactions with a focus on nonlinear optical effects. The project is purely theoretical and will contain both an analytical part and a numerical part. The starting point of the project will be to familiarize yourself with the SSH model and how the single-particle density matrix formalism can be used to describe the optical response in SSH chains. The first task will therefore be to reproduce some of the results from [3]. The next part of the project will be to implement the vector potential is the formalism and investigate the effect this has on the nonlinear response. If time permits, the model can be further enhanced by including the exchange interacting between the electrons which has the prospect of uncovering completely novel insights to the complicated light-matter interactions in solid state materials.

[1] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Solitons in Poly- acetylene, Phys.Rev.Lett. 42, 1698 (1979).
[2] H. W. Streitwolf, Physical properties of polyacetylene, Phys. Status Solidi B 127, 11 (1985).
[3] S. de Vega, J. D. Cox, F. Sols, and F. J. García de Abajo, Strong-Field-Driven Dynamics and High-Harmonic Generation in Interacting One Dimensional Systems, Phys. Rev. Res. 2, 013313 (2020).
[4] C. Jürß and D. Bauer, High-Harmonic Generation in Su-Schrieffer-Heeger Chains, Phys. Rev. B 99, 1 (2019).
[5] L. Jelver and J. D. Cox, Electron-Induced Nonlinear Dynamics in Atomic Chains, Phys. Rev. Res. 5, L022015 (2023).