Laboratoire ESYCOM

Université Gustave Eiffel

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Internship position – Master student

Investigation of Higher Harmonics Scattering from Perovskite Surface using Nonlinear Bond Model

Context

Perovskite is a strong candidate of future solar cell energy generation as well as for next generation of photodetectors. The performance of perovskite based photodevices depends among others on understanding their molecular structure at the nanoscale. Nonlinear optics can be applied to study the Perovskite molecular orientation at this level with the help of rotational anisotropy spectroscopical (RAS) measurement.

This work focuses on developing a nonlinear bond model to investigate higher harmonic generation such as second harmonic generation (SHG) and third harmonic generation (THG) from perovskite surface using a novel and state of the art nonlinear hyperpolarizability bond model. Previous research using the nonlinear bond model were very successful in investigating surface structural properties in semiconductor structures such as silicon in 2014 [1], zincblende in 2016 [2], and wurtzite semiconductors in 2019 [3].

Very recently we have also studied the nonlinear tensor responsible for SHG in perovskite structures [4]. This work was performed by intense collaboration with Dr H. Hardhienata from department of physics of Bogor University Indonesia which need a high self-management skill (to be rigorous, organised, etc.).

Main missions

The focus of this research is to develop further the nonlinear bond model (see **Fig. 1**) to account for different phases of perovskite. At the moment the model only accounts for SHG of the tetragonal perovskite structure [4] but it is well known that perovskite structures can undergo phase transition at different temperatures. Therefore, the aim is to determine the bond vector orientation for the other Perovskite phases as well as explore the possibility for investigation of third harmonic generation (THG) from within the Perovskite bulk. If successful, the results will be reported in a reputable scientific peer review journal.

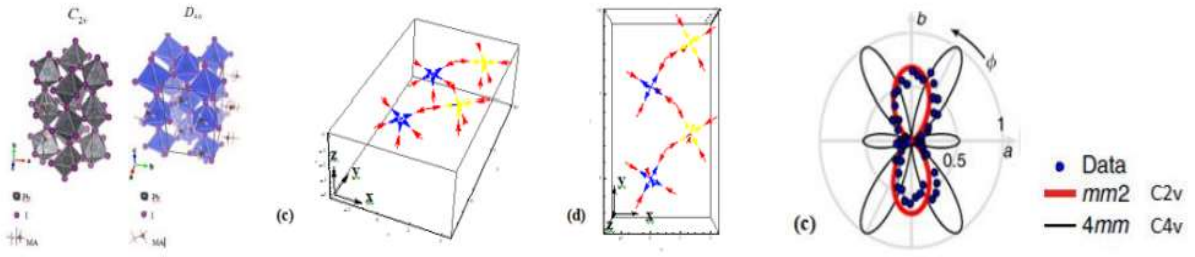

Fig. 1. Perovskite surface structure (left), reduced bulk bond vector (middle) and model outcome (will be like -estimation)

Expected profile:

Knowledge

- Basic Solid-state physics
- Basic on optics (nonlinear optics is a plus)

Knowhow

- Wolfram Mathematica Programming (can be learned afterwards)
- Matlab or C/C++ (optional)
- Phyton (optional)

Location :

Conservatoire National des Arts et Métiers

292 rue Saint-Martin – Paris 75003

Duration :

The duration of this master internship is 5 months. Possible to be reduced to 4 months or extended to 6 months.

Contact:

Salim FACI : salim.faci@lecnam.net (maître de conférences ESYCOM)

References :

1. Adalberto Alejo-Molina, Hendradi Hardhienata, Kurt Hingerl: Simplified Bond Hyperpolarizability Model of Second Harmonic Generation, Group Theory and Neumann's Principle. Journal of the Optical Society of America B **31** (2014)
2. Hendradi Hardhienata, Adalberto Alejo-Molina, Cornelia Reitböck, Andrii Prylepa, David Stifter, Kurt Hingerl: Bulk dipolar contribution to second-harmonic generation in zincblende. Journal of the Optical Society of America B; **33**(195):201(2019)
3. Hendradi Hardhienata, Ignu Priyadi, Husin Alatas, M. Danang Birowosuto, and Phillipe Coquet. Bond Model of SHG in ZnO(0001) using Twin Boundaries. , J. Opt. Soc. Am. B., **36**, 4:1127 (2019)
4. Hendradi Hardhienata, Salim Faci, Adalberto Alejo-Molina, Mohammad R. Priatama, Husin Alatas, and Muhammad D. Birowosuto "*Quo Vadis* Nonlinear Optics? An Alternative and Simple Approach to Third Rank Tensors in Semiconductors" *Symmetry* 14, no. 1: 127, 2022. https://doi.org/10.3390/sym14010127