



Colloquium

Department of Engineering and System
Science,

Institute of Nuclear Engineering and Science,
National Tsing Hua University

非線性光學晶體的第一原理材料設計 First-Principles Materials Design of Nonlinear Optical Crystals

In this talk, the following content will be presented:

Second Harmonic Generation (SHG) is a popular method to achieve frequency conversion (doubling) for laser beam, therefore enrich available wavelength (frequency) spectrum of laser source. Special crystals that can perform SHG is precious due to the importance of potential applications of wide variety kinds of new laser wavelengths. Computational methods has become a indispensable tool in materials sciences, which is very true as well in the field of NLO crystals research. In this talk, I will introduced some basic idea of First- principles Computational Materials Sciences Method, focusing the so-called planewave pseudopotential DFT (Density Functional Theory) based method, the code used is CASTEP. I will also explain those desired properties of a successful SHG NLO crystal, and how they can be studied computationally, followed by showing audiences special tools we developed to gain further understanding of general mechanism and to search for new materials. The information of CASTEP can be found from its official website and my teaching/course website. Options exist to use these powerful software free of charge.

15:30-17:00, Wednesday, December 6th, 2023

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- 台北市人，現居淡水
- 服務於淡江大學物理學系、並同時在台灣大學材料科學與工程學系兼課
- 1990年畢業於淡江大學，獲物理與數學雙主修學士學位（共修業六年）
- 1991年留學英國，受業於 Volker Heine 教授門下
- 1995年獲劍橋大學博士學位，並釋出第一代 CASTEP 層勢資料庫，附隨MSI公司Cerius²軟體全球發行
- 使用CASTEP已30逾年
- 為 Materials Studio CASTEP Psudopotential 資料庫的主要作者，自1995年起至2015年發展了共四個世代
- 持續開發材料物性及化學鍵分析工具，配合CASTEP進行材料之線性與非線性光學性質計算
- 入選 史丹佛大學團隊今年公佈之「2022 全球前 2% 頂尖科學家（World's Top 2% Scientists 2022）」