APPLYING RAMAN TO UNDERSTAND WHERE BORON GOES IN LONG AFTERGLOW CERAMICS?

- STUDENTS / UNIVERSITIES
  DEFNE ÇİRCİ
- SUPERVISOR(S)
  CLEVA OW YANG

Sabancı Üniversitesi

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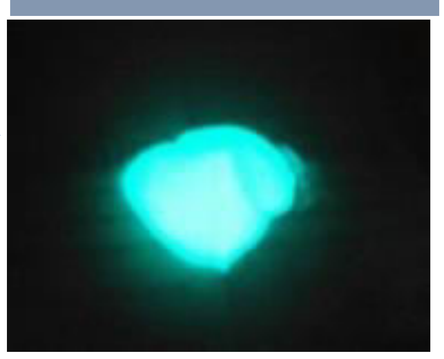
PURE PROGRAM FOR UNDERGRADUATE RESEARCH

AIM

We are trying to understand the structural changes induced by boron in Strontium Aluminates via Raman spectroscopy which is challenging to determine due to multiphase structure. We are using computational analysis to get more accurate results

ROOM LIGHTENING

AFTER UV ILLUMINATION



WHAT

Eu^{+2} and Dy^{+3} and

30% mol boron oxide coactivated Strontium Aluminate

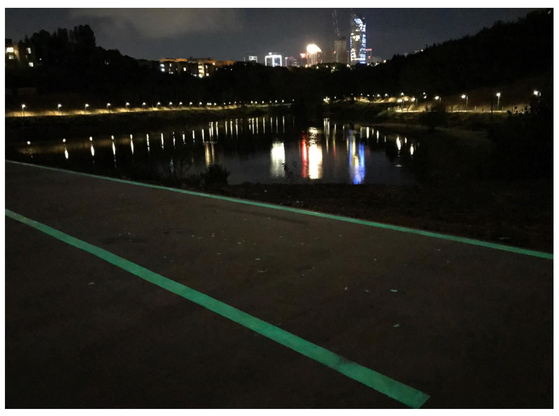
WHERE

Exit signs, pedestrian crossings, luminous vest, lightening of roads..

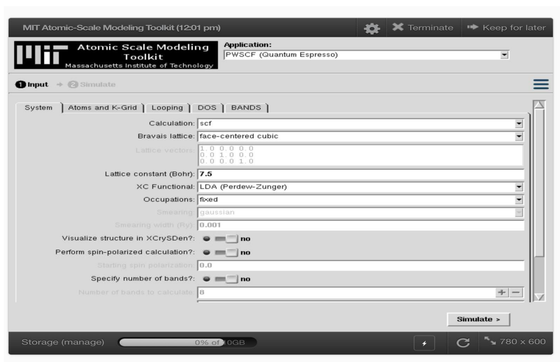
WHY

It can be a candidate for zero energy consumption lightening.

Eu+2, Dy+3 and B induced strontium aluminates can exhibit green afterglow up to 14 hours, whereas without B, it can exhibit only 2-3 minutes afterglow.



Dr. Nuri Solak of Kupfer Ltd

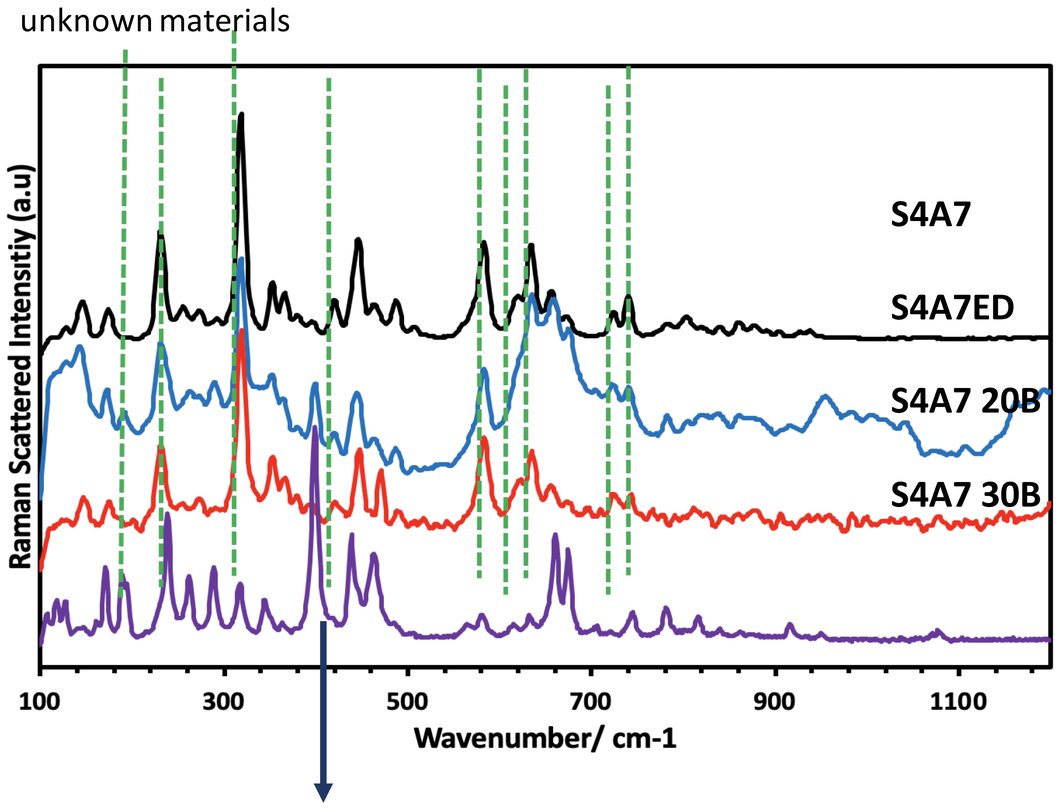


HOW

Using theoretical calculation of vibrational mode frequencies to determine the location of B in the structure using Quantum Espresso

RAMAN SPECTROSCOPY

- Energy absorbed from the inelastically scattered light distorts the random motion of the molecules and make them move together
- Molecules absorb light of specific frequencies that are characteristic to their structure
- Different vibrational modes -spectral footprints- can be used to identify unknown materials



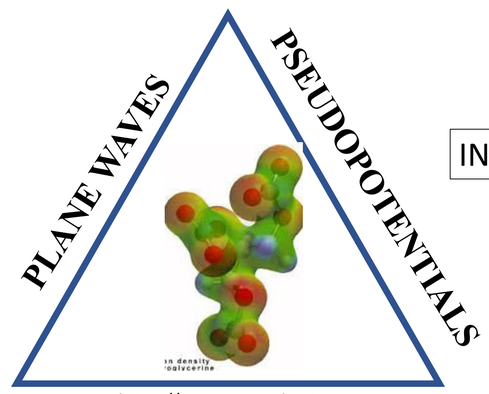
MULTI-PHASE STRUCTURE, TYPICAL OF SYNTHESIZED CERAMICS

QUANTUM ESPRESSO

«IF WE UNDERSTAND THE ELECTRONS, WE CAN UNDERSTAND EVERYTHING»

Periodic
↓
the wave function is periodic

Square of the wave function
↓
probability of the electrons being found in certain locations



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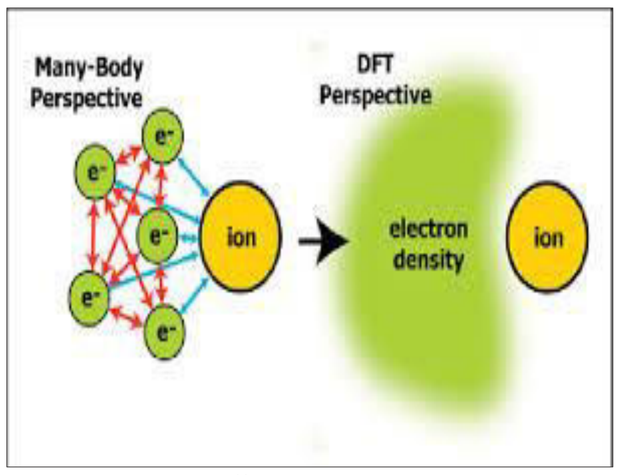
DENSITY FUNCTIONAL THEORY

Total energy is a functional of the electron density

ELECTRONS

INNER CORE

VALANCE
↓
play a significant role in the chemical binding of atoms



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- more easily handled than the complicated wave function in the Schrödinger equation
- possible to set up equations whose solutions give the system's electron density and energy
- Simple
- applied to fairly large molecules

CONCLUSIONS

- Quantum Espresso is a useful tool for microscopic understanding and with the help of DFT, we can use it find position of the B atoms in the large and complex structures like dopant induced Strontium Aluminates while having a low time complexity.
- Role of necessary functions like &control, system, electrons, atomic species and positions for analysing the Raman Data are learned and used for simpler molecules.
- In order to find the best approximation, problems which are listed below should be analysed deeply.

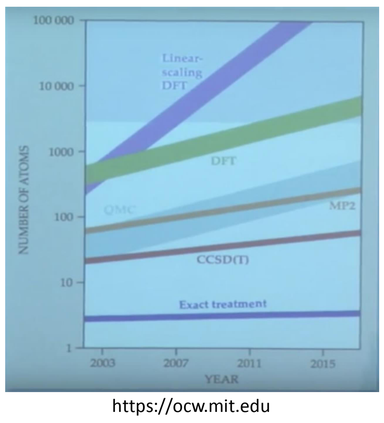
Which atoms are involved?

Where are the atoms sitting?

How big is the unit cell?

At what point do we cut the basis off?

When to exit the self consistent loop?



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