Naughton REU Application

SUMMER INTERNSHIP OFFER OF TRAINING FORM SUMMER 2022

Proposer details:	
Title:	Computational study of the optical properties of MOFs to design new light emitting materials.
Name:	Davide Tiana
Email:	davide.tiana@ucc.ie
Website:	https://orcid.org/0000-0002-3627-1561
If your grade does not allow you to supervise students, please supply the name of support PI:	

Student required:	
Specify any previous training / experience the student should have:	
No previous training in comp chem required.	
Study level (3rd year, 4th year)	3rd or 4th
Any other requirements:	Basic knowledge of solid-state physical/chemistry (e.g. band structure)

Traineeship offered:
Brief job description: (please include (1) type of work, (2) what student should hope to achieve at end of the process, (3) who will supervise student on daily basis (post-doc etc.))
Our society relies heavily on lighting. Lighting accounts for more than 10% of the electricity consumption for the residential and commercial sector, whilst public street lighting costs several millions of euro's to city councils. Improvements in the efficiency of light devices will have a major impact on society for both practical (better illumination, longer battery life) and economic reasons (saving a large amount of money). This project is focused on finding new, more-efficient materials for light emission. 1) The student will study the opto-electronic properties of Metal-Organic Frameworks (MOFs) for Light Emission Diodes. At the beginning of the project the student will learn how to use computational chemistry software (e.g. quantum espresso or CP2K) and will perform a literature review on MOFs for opto-electronic properties. This induction will be followed by a computational study of the optical properties of a MOF (e.g. ZIF-8). The student will 1st calculate the band structure of the pristine material and then will simulate the effect of

doping on the opto-electronic properties.

2) Leaning outcome:
At the end of the project the student will be able to:

- use computational software to simulate and study opto-electronic properties of materials.
- explain the opto-electronic properties of material using band structure. And acknowledge the importance of doping to improve materials properties.
- rationalize the structure opto-electronic properties of MOFs understanding how these can be tailor-made.

3) The PI will supervise and train the student.

Link to research group or supervisor webpage:	https://orcid.org/0000-0002-3627-1561
Location of lab:	Cork Comp Chem and Programming Lab, Kane Building, UCC, College Road Cork.

Working hours:	
Number of Weeks offered:	8
Hours per week:	36
Earliest Start Date possible:	01/05/2022
Latest End Date possible:	31/08/2022