工学系WINGS産学協創教育推進基金

第411回GMSI公開セミナー／第156回WINGSセミナー

# What can we Learn about CVD and Nanomaterial Growth using Computational Approaches?


## Professor Alister Page

Computational & Physical Chemistry
College of Engineering, Science & Environment
The University of Newcastle


**Date: Wednesday, January 10, 2024 15:00-16:30**
**Venue: Faculty of Engineering Bldg. 2, Room 31A**


**Abstract:**

Over the last few decades, catalytic chemical vapor deposition (CVD) has matured as a synthetic technique for producing many low-dimensional inorganic nanomaterials, such as carbon nanotubes (CNTs), graphene, boron nitrides and transition metal dichalcogenides. van der Waals heterostructures comprising these 1D and 2D allotropes have also been recently developed. During this time, Computational approaches have played a critical role in developing our understanding of the structure, properties and growth of these materials. In this talk, I will summarise our own recent contributions to this field, and will discuss how molecular dynamics and quantum chemistry help us understand the chemistry of CVD nanomaterial growth [1,2], nucleation mechanisms of 1D and 2D inorganic nanomaterials [3] and heterostructure stability. I will also discuss our work employing machine learning and graph-neural network approaches for identifying improved heterogeneous catalytic interfaces for CVD nanomaterial growth [4].



**Professor Alister Page**
Computational & Physical Chemistry
College of Engineering, Science & Environment
The University of Newcastle



1. Eveleens, C., Page, A. J., Nanoscale, 9, 1727-1737 (2017). DOI: 10.1039/C6NR08222J
2. McLean, B., Kauppinen, E.I., Page, A. J. Journal of Applied Physics. 129, 044302 (2021). DOI: 10.1063/5.0030814
3. McLean, et al. Journal of the American Chemical Society. 141, 13385-13393 (2019). DOI: 10.1021/jacs.9b03484
4. Li, et al. Journal of Physical Chemistry Letters. 12, 7305-7311 (2021). DOI: 10.1021/acs.jpclett.1c01851


主催：
東京大学大学院工学系研究科専攻間横断型教育プログラム 機械システム・イノベーション（GMSI）
未来社会協創国際卓越大学院（WINGS CFS）
量子科学技術国際卓越大学院（WINGS-QSTEP）
統合物質・科学国際卓越大学院（MERIT-WINGS）
高齢社会総合研究国際卓越大学院（WINGS-GLAFS）
工学系WINGS産学協創教育推進基金


本件連絡先：
東京大学大学院工学系研究科機械工学専攻 教授 丸山 茂夫
GMSI事務局 E-mail: office@gmsi.t.u-tokyo.ac.jp Phone: 03-5841-0696