

# Joint CQSE and CASTS Seminar

Weekly Seminar  
Nov. 4, 2016 (Friday)

TIME Nov. 4, 2016, 14:30 ~ 15:30  
TITLE Computational Material Design of Two Dimensional Materials  
and Their Energy Applications  
SPEAKER Prof. Jer-Lai Kuo  
Institute of Atomic and Molecular Sciences, Academia Sinica  
PLACE Rm716, CCMS & New Physics Building, NTU

## Abstract

Two-dimensional materials have attracted attention from both fundamental aspects and application. In this work, we will present some of our recent effort to using first-principles based computational tools to design two-dimensional materials for energy applications. We have explored new possible ionic two dimensional materials and discover some that have not been synthesized yet<sup>1</sup>. Furthermore, their potential applications to adsorption of Li (for battery and hydrogen storage)<sup>2</sup> and hydrogen evolution reactions<sup>3</sup> are also examined.

[1] Chung-Huai Chang, Xiaofeng Fan, Shi-Hsin Lin, J-L Kuo, *Phys. Rev. B*, **88**, 195420 (2013)

[2] S-H Lin, and J-L Kuo, *Phys. Chem. Chem. Phys.*, **16**, 20763 (2014)

[3] Yun-Wen Chen, Yaojun Du, and J-L Kuo, *J. Phys. Chem. C*, **118**, 20383 (2014)

[4] D. B. Putungan, S-H Lin, and J-L Kuo, *Phys. Chem. Chem. Phys.*, **17**, 11367 (2015)

