Materials for Energy Applications: How Theoretical Modeling Contributes to the Experiment?

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Significant research progress in the field of 2D materials has been made in recent years following the discovery of graphene. Such materials at reduced dimension possess well-known quantum confinement and large surface area, which have significant impact on materials' catalysis properties. One of my recent research focuses is to provide in-depth understanding of material properties at atomic level and develop novel strategies to manipulate the electronic structure of nanomaterials for energy applications via high throughput computer screening and density functional theory approaches.

In this talk, I will present our recent key research findings on (i) predicting 2D MXenes as efficient catalyst for hydrogen evolution reaction [1] as evidenced by experiment[2]; (ii) proposing to strain-modulated chemical reaction [3] which is consistent with most recent experimental findings [4]; (iii) predicting a novel single atom catalyst based on transitional metal decorated graphitic carbon nitride [5] with confirmation from multiple experiments; (iv) predicting the coordination effect between transitional metal and carbon atoms on hydrogen/oxygen evolution reaction [6] as demonstrated by later experimental findings [7]; [v] predicting a metal-free single atom catalyst for N2 fixation [8] for future experimental verification.

References:

[1] Gao *et al.* ***ACS Catalysis*** 7 (2016) 494-500.
[2] Ran *et al.* ***Nature Communications*** 8 (2017) 13907.
[3] Gao et al. ***J. Catalysis*** 332 (2015) 149. Highlighted in Advances in Engineering.
[4] **Science** 352 (2016) 73; 354 (2016) 1031; 363 (2019) 870.
[5] Gao *et al.* ***JACS*** 138 (2016) 6292.
[6] Gao et al. ***Catalysis Science & Technology*** 8 (2018) 996.
[7] Zhang et al. ***Chem*** 4 (2018) 285.
[8] Ling *et al.* ***JACS*** 140 (2018) 14161.