Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Theoretical Study of Electronic and Defect Properties of 2D Alloys BING HUANG, Beijing Computational Science Research Center — Alloy engineering has been developed for modulating the electronic and defect properties of 2D materials. Firstly, we have developed a new concept to modulate the phase diagram of 2D alloys by epitaxial growth, which is the key step to obtain the controllable electronic properties of alloys. Secondly, we have found that homogenous 2D alloys can be applied to tune the electronic properties of 2D materials, making them suitable for various energy related applications. Finally, we suggest a new way to control the defect level positions of 2D materials by alloy engineering.

Bing Huang
Beijing Computational Science Research Center

Date submitted: 11 Nov 2016 Electronic form version 1.4