**Theoretical investigations of the formation Energy and electronic properties of substitutional dopants in WSe2**

Chi-Yuan Chang

Research Center for Applied Sciences, Academia Sinica

Transition metal dichalcogenides (TMDs) are known for their application in semiconductor devices due to their excellent electronic properties and low-dimensional transport. However, the contact resistance of TMDs' devices are high due to severe Fermi level pinning and the difficulties of contact engineering. One solution is doping in the contact region. Therefore, understanding the influence of doping becomes important.

In this work, we adopt first-principles calculations to investigate the formation energy, and electronic properties of selected n-type and p-type substitutional dopants in monolayer WSe$\_2$. First, we calculate the formation energy of each dopant. Second, we focus on Hf, V, Nb, Ta, and P dopants to understand their influence on the electronic structure.