**Fictitious Temperature in TAO-DFT**

Jeng-Da Chai

National Taiwan University

In contrast to the widely used Kohn-Sham density functional theory (KS-DFT), thermally-assisted-occupation density functional theory (TAO-DFT) [J.-D. Chai, J. Chem. Phys. 136, 154104 (2012)] is a density functional theory with fractional orbital occupations given by the Fermi-Dirac distribution (controlled by a fictitious temperature), for the study of large electronic systems with multi-reference character. Owing to its computational efficiency and reasonable accuracy, TAO-DFT has been recently applied to the study of various nanomaterials with multi-reference character (i.e., challenging systems for conventional electronic structure methods). The role of TAO-DFT fictitious temperature and a few interesting results will be presented.