# Optical signatures and fine structures of dark excitons in transition metal dichalcogenide monolayers

**Shun-Jen Cheng**
Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan
e-mail address: sjcheng@mail.nctu.edu.tw

Atomically thin transition-metal dichalcogenide monolayers (TMD-MLs) have recently drawn broad attention because of the extraordinary spin-, valley- and excitonic properties. [1,2] With the combined spin- and valley-degrees of freedom, an exciton in a TMD-ML under photo-excitation exhibits the complex fine structures, composed of the bright exciton (BX) states, and spin-forbidden (SF) and momentum-forbidden (MF) dark states (DXs) as well. Because of the optical invisibility, both of the SF- and MF-dark states are in principle hardly observed and even distinguished in conventional spectroscopies though their impacts on the optical and dynamical properties of TMD-MLs have been well noticed. In this work, we shall report on our theoretical and computational investigation of the excitonic fine structures and the optical signatures of the dark excitons in the temperature-dependent photo-luminescence (TD-PL) spectra of TMD-MLs. The excitonic spectra are calculated by solving the density-functional-theory (DFT)-based Bethe-Salpeter equation (BSE) with the full consideration of both electron-hole direct and exchange Coulomb interactions.[3] As main results, we reveal the distinctive signatures of the SF- and MF-DX underlying in the TD-PL of $WSe_2$-MLs, featured by the quickly rising and slowly descending PL intensities with increasing the temperature at low T~80K and high T~260K, respectively. The computational results agree well with the existing experimental data, [4] and account for the impact of the high lying MF-DX states on the optical properties of W-based TMD-MLs.

**References**

[1] K. F. Mak, C. Lee, J. Hone, J. Shan, and Tony F. Heinz, Phys. Rev. Lett., 2010, **105**, 136805.
[2] D. Xiao, G. B. Liu, W. Feng, X. Xu, and W. Yao, Phys. Rev. Lett., 2012, **108**, 196802.
[3] G.-H. Peng, P.-Y. Lo, W.-H. Li, Y.-C. Huang, Y.-H. Chen, C.-H. Lee, C.-K. Yang, and S.-J. Cheng, Nano Lett., 2019, **19**, 2299.
[4] X.-X. Zhang, Y. You, S. Y. F. Zhao, and T. F. Heinz, Phys. Rev. Lett., 2015, **115**, 257403.