Light emission in 2D materials studied by STM-induced luminescence

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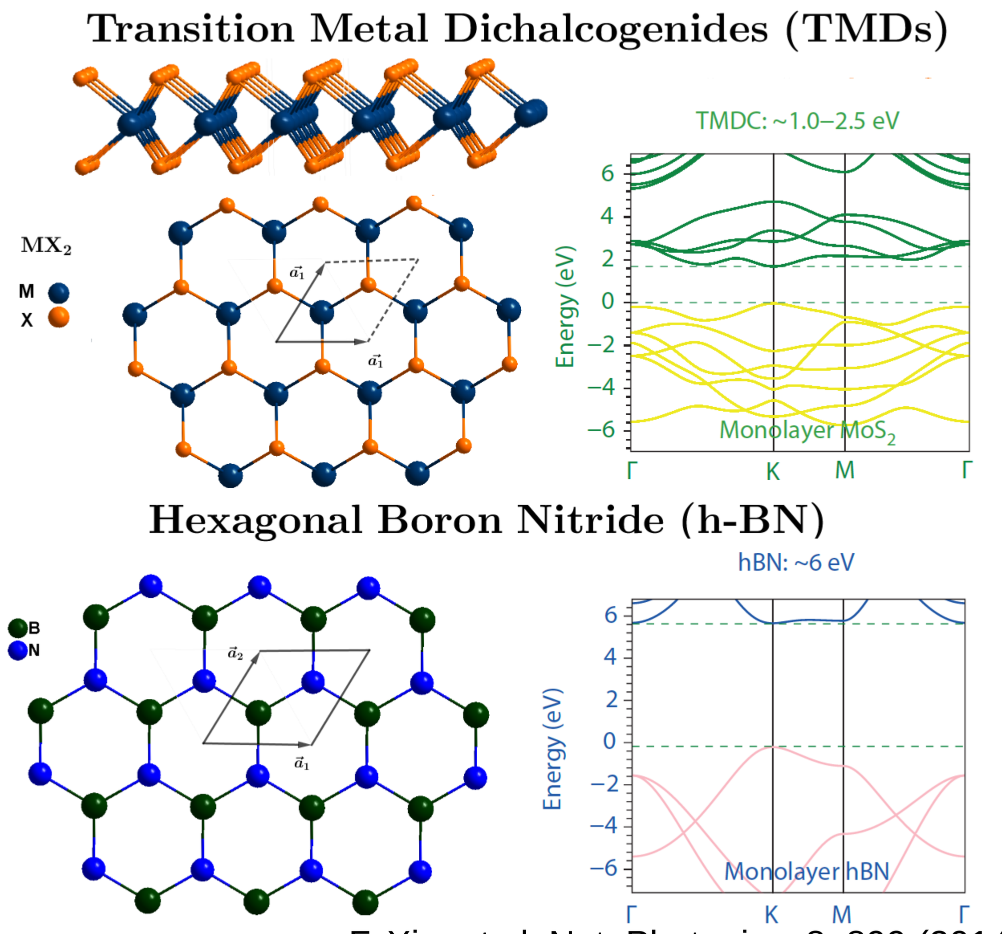
Two-dimensional (2D) materials graphene-like, such as hexagonal boron nitride (h-BN) and semiconducting transition metal dichalcogenides (TMDs), e.g., MoS_2, WS_2, and WSe_2, have been studied extensively in the last years due their great and tunable optical properties [1]. The effect of point defects in the structure of these kind of materials also have been investigated recently due the fact that the optical properties of h-BN as well as of TMDs can be modulated by defect engineering [2]. Point defects confine electronic levels within the band gap of the material, thus point defects lead to stable and robust single photon emitters (SPEs) in h-BN [3], and in the case of TMDs, defect-bound excitons may behave like SPEs [4]. A SPE is a critical element for quantum information [5]. Some works have reported that defects enhance the luminescence of TMDs as well [6].

In order to understand the structural, electronic and optical properties of individual point defects in 2D materials, we will make to use of a scanning tunneling microscope (STM) accoupled to an efficient light detection system to carry out STM-induced luminescence [7] experiments at low temperature and in ultra-high vacuum. Hence, we will use the STM to obtain images with atomic resolution to identify defects in the structure, measure STS curves to study the electronic properties of defects, and detect the light emitted by the recombination of charge carriers close to defects. As a preliminary characterization of 2D materials, AFM measurements and photoluminescence experiments are being performed to study the morphology and optical activity of h-BN and some TMDs.

Introduction

Understanding the effect of structural defects on the electronic and optical properties of 2D materials is important to develop strategies to modulate their properties by defect engineering and tailor 2D materials with new functionalities which may be useful in some applications. Semiconducting TMDs and h-BN have received extensive attention in the las year due their great electronic and optical properties.

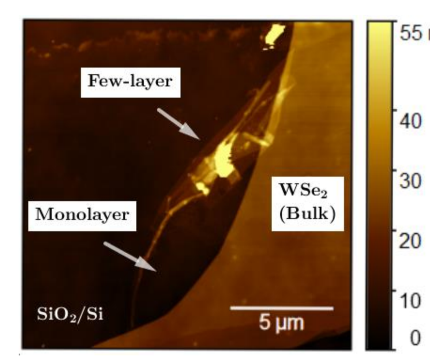


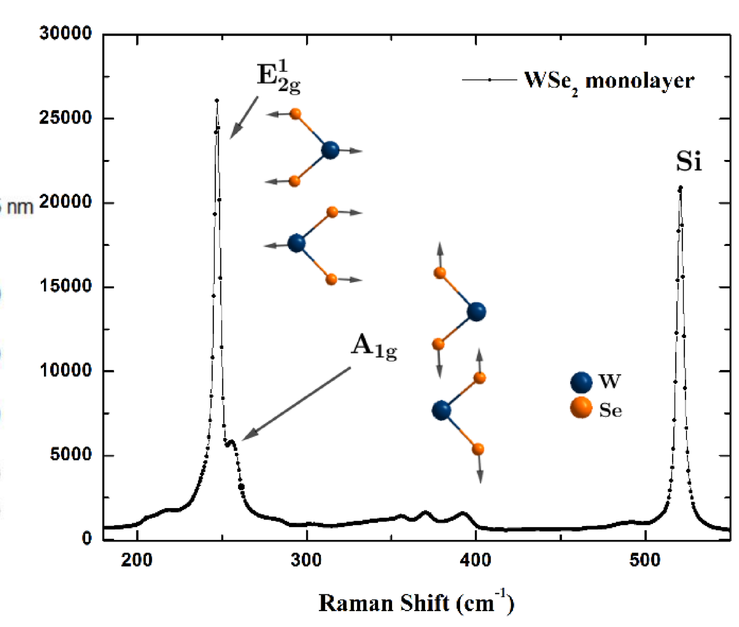
F. Xia, et al. Nat. Photonics. 8, 899 (2014).

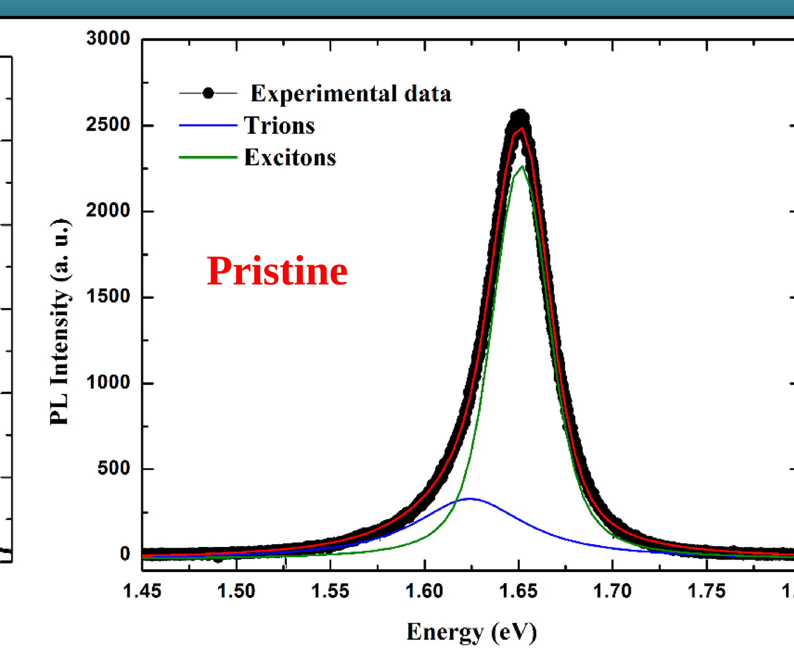
Structural and optical properties of point defects in 2D materials

Preparation and preliminary characterization of monolayer of WSe_2 and flakes of h-BN. The monolayer of WSe_2 has been mechanically exfoliated on SiO2/Si and characterized by AFM, Raman, and PL spectroscopy. Experiments to create point defect by ion implantation are being planed. In the case of h-BN, point defects are been created by thermal treatment and studied by PL spectroscopy.

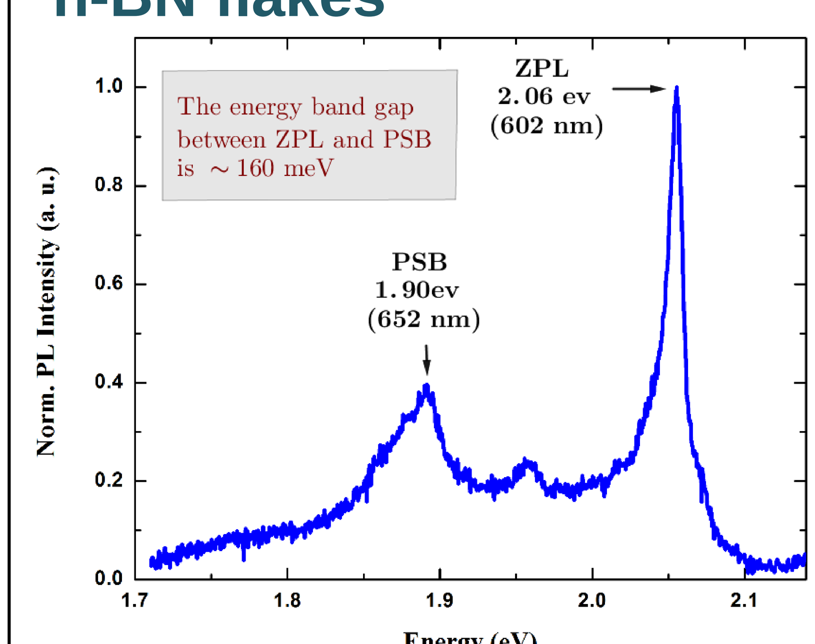
WSe_2 monolayer

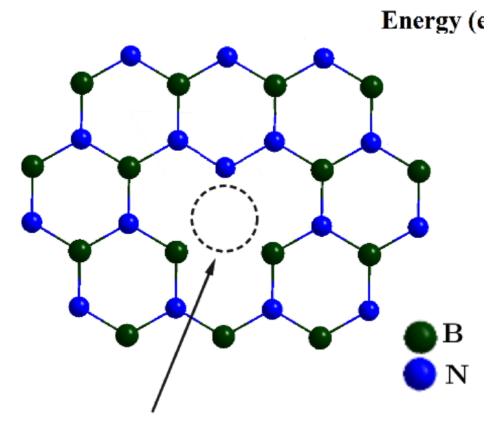






h-BN flakes



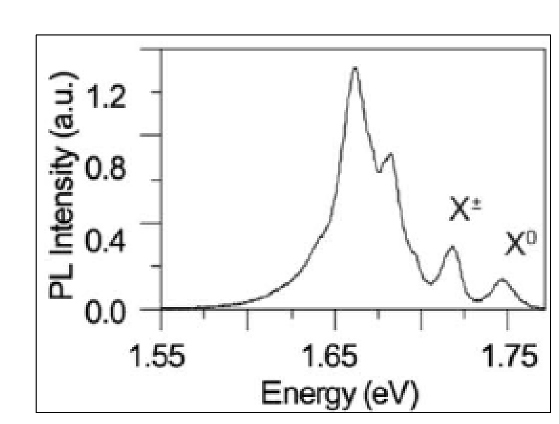


Point defect in the structure of h-BN. Nitrogen vacancy and a boron atom substituted to a nitrogen vacancy [3].

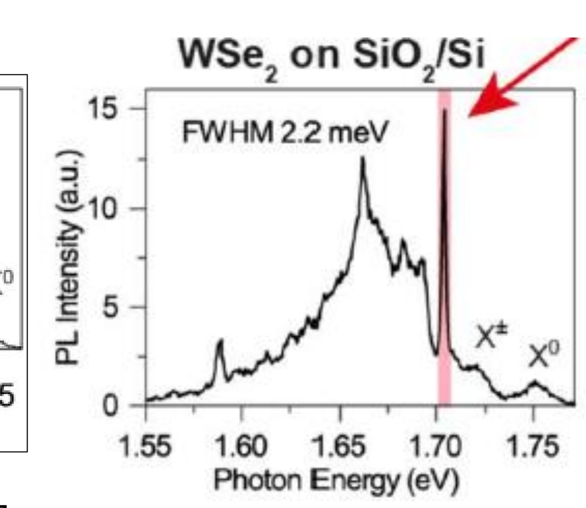
Defects in WSe_2 and h-BN

Several works have reported that point defects in h-BN place electronic levels into the band-gap that lead to electronic transitions that result in single photo emission source.

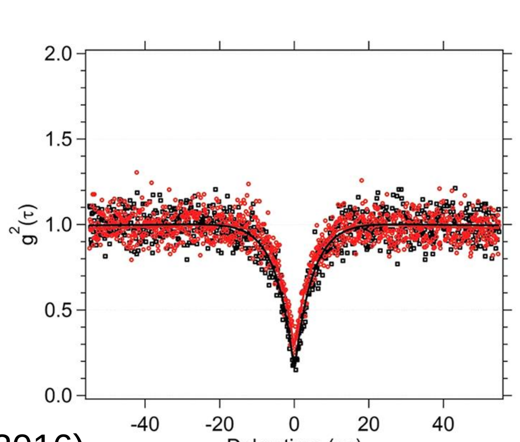
In the case of WSe_2 and other semiconducting TMDs, point defects (vacancies, impurities) introduce deep and localized states into de band-gap that act as trap to non-radiative excitonic recombination leading to an enhancement of luminescence. On the other hand, defect-bound excitons may behave like SPEs.



P. Tonndorf, *et al*. Optica 2, 347 (2015).



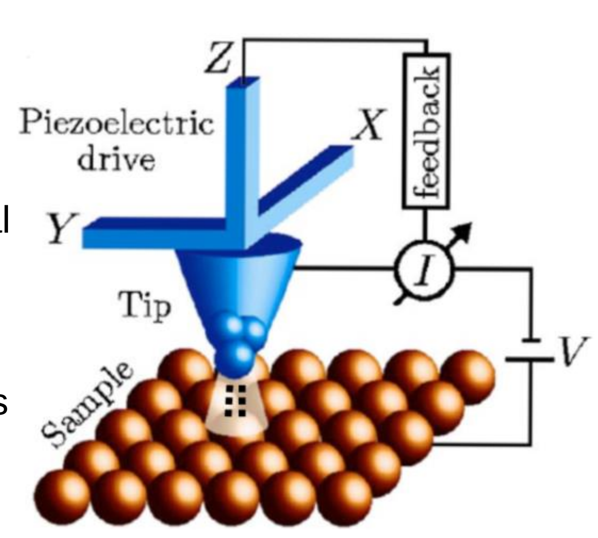
Single photon emitter (SPE)



T. T. Tran, *et al*. Nano, 10 (8), 7331 (2016).

STM-Induced Luminescence

Scanning tunneling microscopy (STM) is a powerful technique that allow to study the structural and electronical properties of conducting or semiconducting surfaces with atomic resolution. In STM, a bias voltage is applied between the tip and sample and a tunneling current is measured.

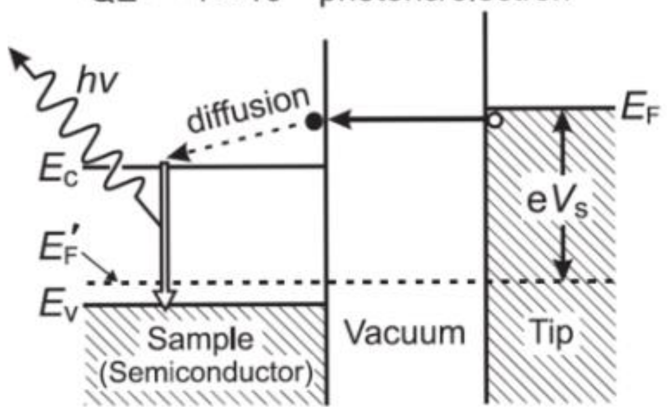


O. Fischer, *et al*. Rev. Mod. Phys. 79, 353 (2007).

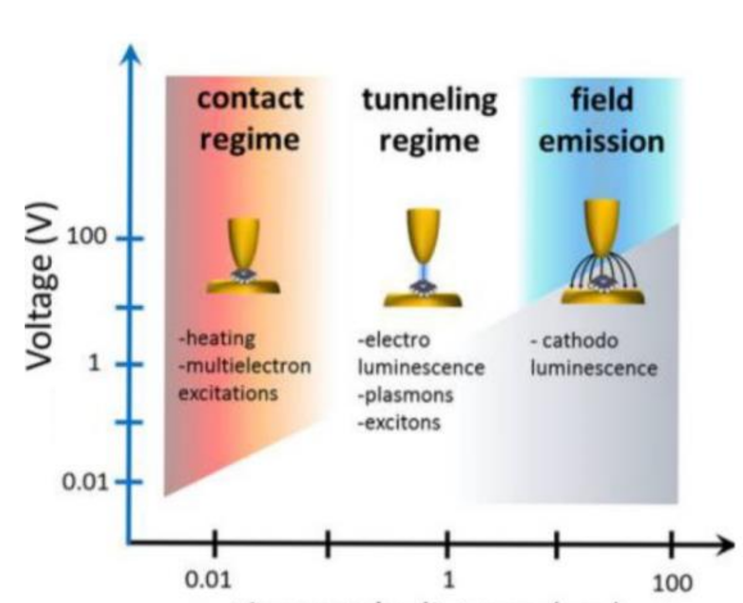
The tunneling current can induce the light emission from the sample. This make possible to study the optical properties of the sample in a local way using the high spatial resolution of STM.

Electron-hole recombination

QE=~1×10^{-4} photons/electron

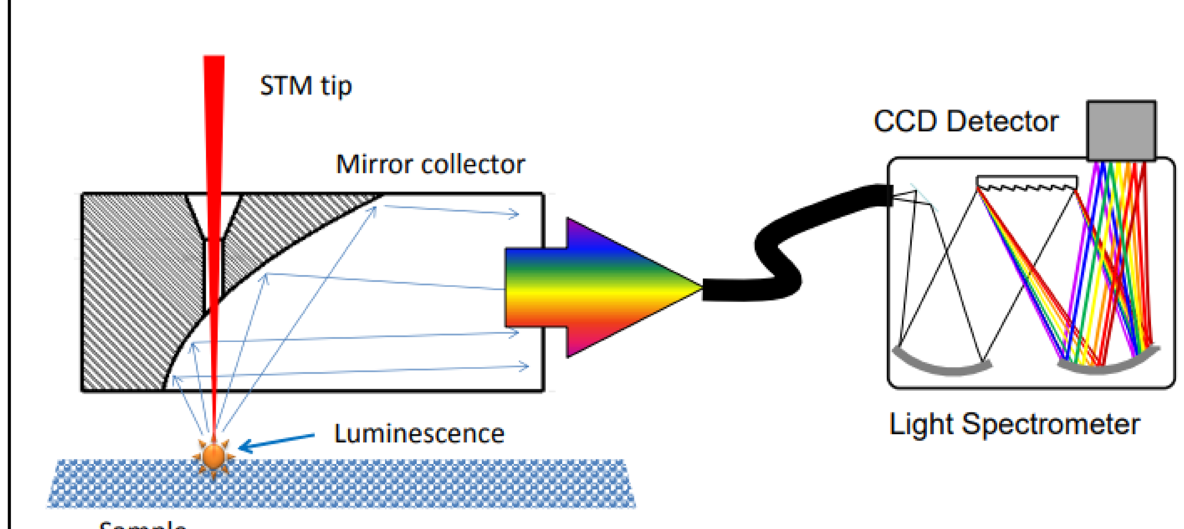


M. Sakurai, *et al*. Appl. Phys. A 80, 1153 (2005)



K. Kuhnke, *et al*. Chem. Rev. 7, 5174 (2017).

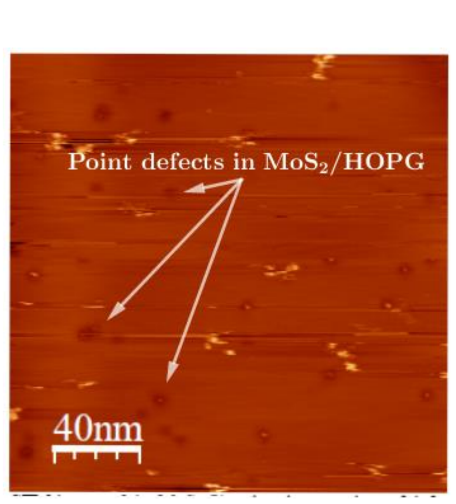
STM-Induced Luminescence experimental setup

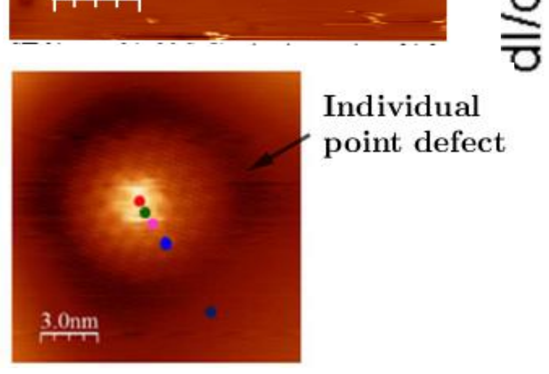


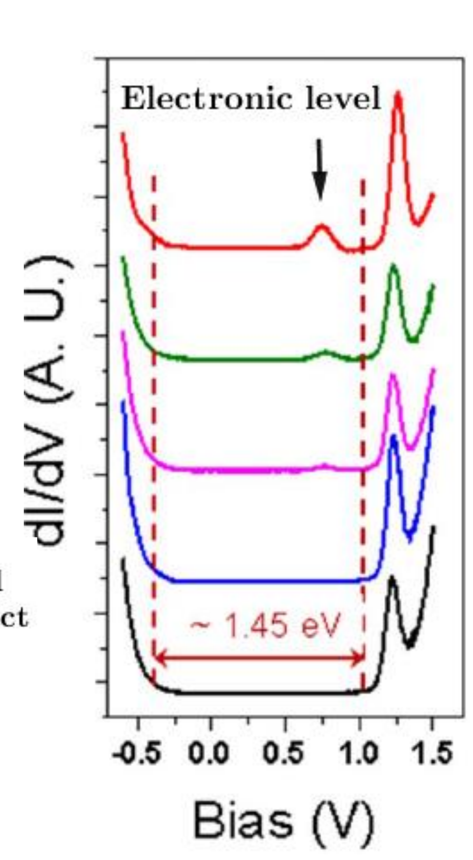
Our experimental system will use a patented solution for high collection efficiency and nearly lossless coupling to the spectrometer while preserving high spatial resolution [8,9]

STM-Induced Luminescence in 2D materials

STM together with STS (scanning tunneling spectroscopy) can be used to image the atomic structure in order to identify defects on the sample surface, and investigate the local density of states to obtain information about the electronic structure and defect electronic levels.



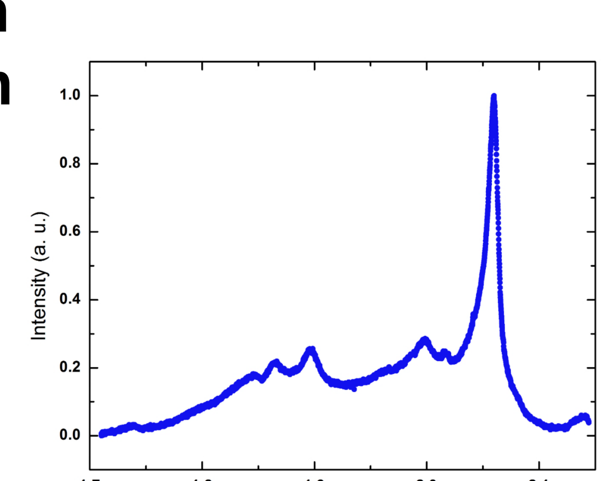




STS measurements

$$\frac{dI}{dV} \propto \exp\left[-2z\sqrt{\frac{m_e}{\hbar^2}\left(\frac{\phi_t+\phi_s}{2}\right)}\right]\rho^t(0)\rho^s(eV,x,y).$$

Emission spectrum



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