Hot luminescence or Raman scattering in monolayers of $MoSi_2N_4$

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Monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), *e.g.* MoS_2 and WSe_2, have been demonstrated to carry the spin-like degree of freedom known as valley pseudospin due to the optical bandgap located at the $K^{\pm}$ points of their hexagonal Brillouin zone [1]. Recently, MLs of the MSi_2Z_4 family (M = Mo, W; Z = N, P, As, Sb), which form a new class of hexagonal non-centrosymmetric materials hosting extraordinary spin-valley physics, have been discovered [2].

In this work, we investigate the optical response of the $MoSi_2N_4$ ML, grown using chemical vapor deposition on Si/SiO_2 substrate [3], with the aid of photoluminescence (PL) performed in a wide range of temperature (5 – 300 K) and first principles calculations.

The relative PL spectra, calculated as the difference between the PL spectra measured on the ML and on the Si/SiO_2 substrate, as shown in the Figure. $MoSi_2N_4$ MLs are semiconductors with an indirect band gap of about 1.94 eV at 300 K. However, the excitation of the PL spectra with high energies of 3.06 eV or near to the band gap of 1.96 eV does not give rise to a measurable signal either at 300 K or at 5 K. Nevertheless, a significant PL is apparent under excitation close to the so-called A and B direct transitions in the $K^{\pm}$ valleys [3]. The obtained relative spectra are combined of two types of emission, *i.e.* a broad band with linewidths of ~200 meV, on top of which a series of narrow peaks emerges. Consequently, it is difficult to decompose this emission to Raman scattering or hot luminescence, since the ratio between the resonantly enhanced Raman signal and the optical recombination at the $K^{\pm}$ points is unknown. At T=5 K, only the Raman peaks are seen, which were ascribed to phonon modes using the calculated phonon dispersion spectrum.

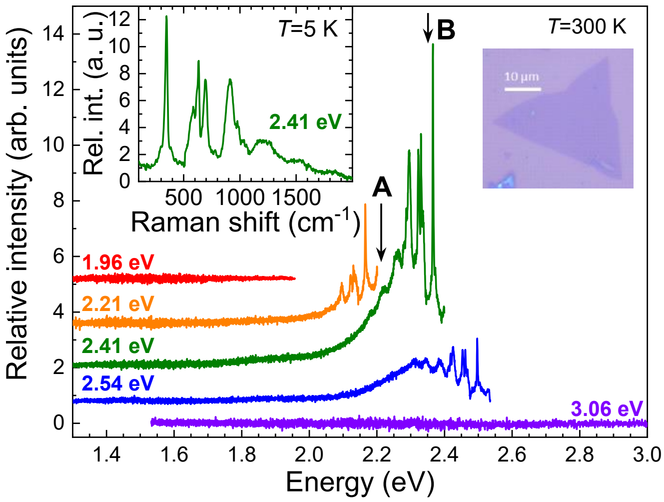

Figure Relative PL spectra of $MoSi_2N_4$ ML under different excitations. The insets show the spectrum at 5 K and the optical image of the studied ML.

Our results are the spore of research devoted to the MLs of the $MoSi_2N_4$ family, which properties locates them as ideal candidates for valleytronics, in line with S-TMD MLs.

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[2] T. Woźniak, *et al.*, *Small* 2206444 (2023).
[3] Y.-L. Hong, *et al.*, *Science* 369, 670 (2022).