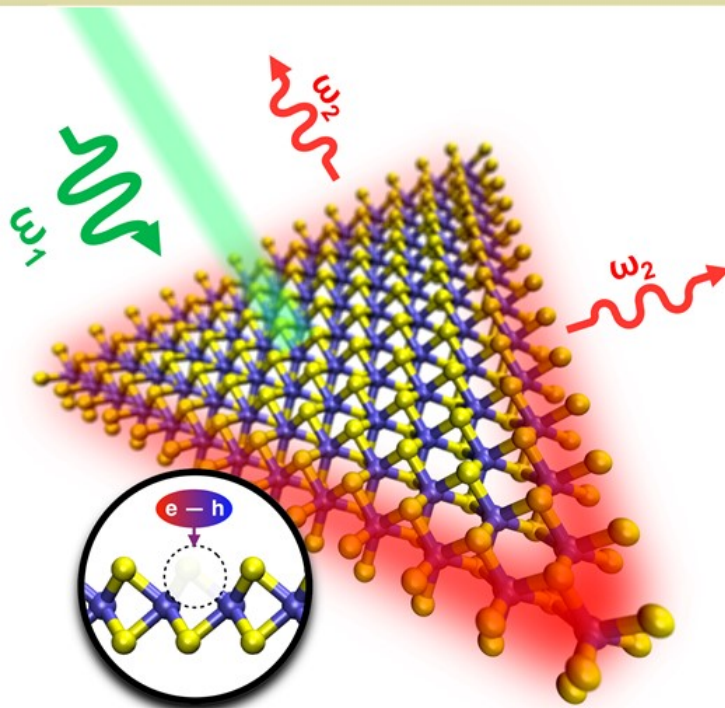


MIP: 2D Crystal Consortium
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Excitons bound to defects

Identifying crystal defects in a 2D crystal usually requires an electron microscope to directly resolve atomic details, a complex and time-consuming process on expensive equipment that can damage the sample under electron irradiation. By establishing a correlation between the modified optical response and certain defects, the MIP team and collaborators have demonstrated a quick and non-destructive method of identifying defects in 2D crystals. The reason for this correlation is identified through first-principles calculations: electrons trapped by sulfur vacancies – the absence of a sulfur atom – have energies that are forbidden for electrons in defect-free regions, and therefore emit light at wavelengths different from that of the latter.



An international collaboration with Brazil CNPq/PDE (249070/2013-8) and FAPEMIG.



DMR DIVISION OF
MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Carozo, Wang, Fujisawa, Carvalho, McCreary, Feng, Lin, Zhou, Perea-López, Elías, Kabius, Crespi, Terrones, Penn State, Universidade Federal de Minas Gerais

Figure Title: Identifying Defects.

Figure Caption: An atomically thin WS₂ flake is shown to be excited by a laser and emit light at a different wavelength at the three edges of the triangular flake. The inset illustrates an electron-hole pair being trapped at a sulfur vacancy site.

What Has Been Achieved: A photoluminescence feature has been identified as excitons bound to charged sulfur vacancies in 2D WS₂.

Importance of Achievement: The study identifies a fast, inexpensive, and non-destructive characterization method to assess the quality of 2D transition metal dichalcogenide crystals.

Unique Features of the MIP That Enabled Project: Close collaboration between synthesis, characterization, and theory efforts.

Publication: V. Carozo, Y. Wang, K. Fujisawa, B. R. Carvalho, A. McCreary, S. Feng, Z. Lin, C. Zhou, N. Perea-López, A. L. Elías, B. Kabius, V. H. Crespi, and M. Terrones, "Optical identification of sulfur vacancies: Bound excitons at the edges of monolayer tungsten disulfide", *Sci. Adv.* 3, e1602813 (2017).