

Electronic Spectroscopy of Atomic Defects in Molybdenum Disulfide under Ambient Conditions

J. R. Evans,¹ D. A. Garibay,² A. N. Kuhls,² and M. Z. Baykara²

¹ *Department of Materials Science and Engineering, University of California Merced, 5200 North Lake Road, Merced, CA 95343, USA*

² *Department of Mechanical and Aerospace Engineering, University of California Merced, 5200 North Lake Road, Merced, CA 95343, USA*

Two-dimensional transition metal dichalcogenides (2D-TMDs) are promising candidates for next-generation, nanoscale electronic devices due to their profound optoelectronic properties (e.g., direct and tunable bandgaps) [1]. However, these materials host atomic-scale defects (e.g., vacancies, substitutions, *etc.*), introducing electronic heterogeneities that can either enhance or hinder device performance [2], [3]. Thus, characterizing atomic defects within 2D-TMDs is essential for nanoscale device implementation.

Current-voltage (I - V) spectroscopy via conductive atomic force microscopy (C-AFM) characterizes electronic properties under ambient conditions [4]. Thermal drift makes this method unsuitable, reducing confidence in assigning electronic features to specific defects. We present an alternative approach on molybdenum disulfide (MoS_2), a representative 2D-TMD, that overcomes thermal drift [5]. Consecutive current maps are collected at various bias voltages, enabling direct assessment of electronic features for defects spanning single atomic sites to several nanometers. Spectroscopy data allows sorting defects into distinct groups, leading to their chemical identification.

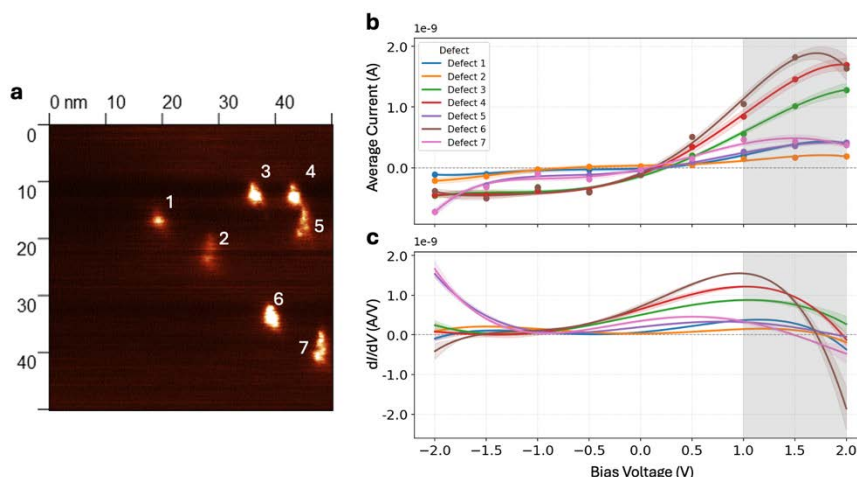


Figure 1. (a) C-AFM current map of MoS_2 defects; bias voltage: +2 V. (b) Averaged current plotted as a function of bias voltage associated with all seven defects in (a). (c) Derivatives of fitted curves in (b), producing dI/dV - V curves for defects in (a). Shaded region in (b) and (c) indicates potential tip change, causing an unexpected drop in slope.

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- [2] Y. Zhu *et al.*, “Point defects in semiconductors: Friends and foes for quantum technologies,” *MRS Bull.*, vol. 51, no. 5, pp. 615–629, May 2026, doi: 10.1557/s43577-026-01095-x.
- [3] B. Kumral *et al.*, “Mechanically reliable and electronically uniform monolayer MoS_2 by passivation and defect healing,” *Nat. Commun.*, vol. 16, no. 1, p. 7105, Aug. 2025, doi: 10.1038/s41467-025-62370-0.
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- [5] J. R. Evans, D. A. Garibay, A. N. Kuhls, and M. Z. Baykara, “Electronic Spectroscopy of Atomic Defects in Molybdenum Disulfide under Ambient Conditions,” *ACS Omega*, in press, 2026.

Supplementary Information

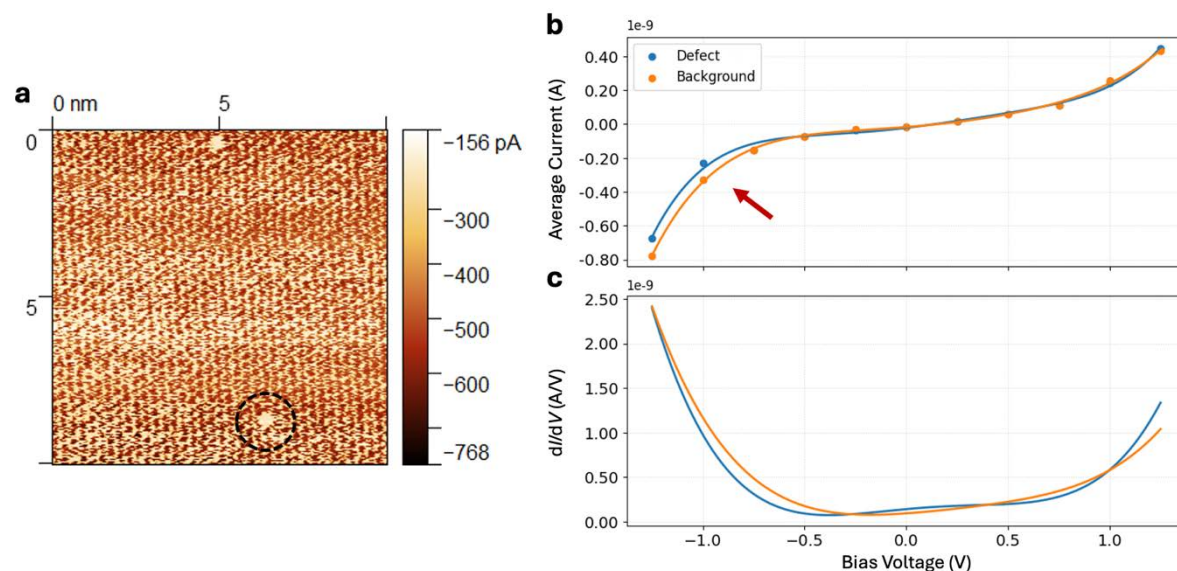


Figure 2. (a) A $10 \times 10 \text{ nm}^2$ C-AFM current map on MoS_2 recorded at a bias voltage of -1 V , where two point defects are detected. (b) Average current plotted as a function of the bias voltage for the point defect highlighted by the dashed black circle in (a) (blue), as well as a non-defective (background) region in its vicinity (orange). A deviation of current on the defect from the background signal is detected at increasingly negative voltages (red arrow). (c) The derivatives of the fitted curves from (b), in the form of dI/dV - V curves for the defect (blue) and the background (orange).

* Results associated with this abstract are detailed in the following arXiv pre-print (in press at *ACS Omega*): <https://arxiv.org/abs/2604.23391>