Defect-Mediated Tuning of Electronic and Magnetic Properties of CrSBr

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Bulk CrSBr is a van der Waals semiconducting material that has recently attracted significant attention due to its intrinsic band gap, long-range magnetic ordering, and pronounced electronic anisotropy. [1,2] In addition to these intrinsic properties, it has been experimentally demonstrated that the properties can further be tuned by ion and electron irradiation in the transmission electron microscope (TEM). [3,4] We employ first-principles calculations to investigate the energetics and properties of point and line defects (e.g., edges) in monolayer CrSBr. We analyze defect formation under electron beam in the TEM by evaluating atomic displacement thresholds and calculating displacement cross-sections as functions of electron energy within the McKinley-Feshbach formalism. Furthermore, we explore the electronic and magnetic properties of finite-width nanoribbons oriented along the a, b, and d crystallographic directions. Our results reveal that nanoribbons along a direction are more stable than those along b, while cutting along d produces the most stable ribbons in the Cr-poor limit. [5] The electronic structures of CrSBr nanoribbons strongly depend on both orientation and width, with the most stable edges exhibiting half-metallic behavior. Finally, we examine the effects of Cl substitution on the electronic and vibrational properties of $CrSBr_{1-x}Cl_x$. These findings provide fundamental insights into defect-mediated tunability in CrSBr systems and open new avenues for their application in spintronic devices.[6]

[1] N. Wilson, K. Kee, et al., *Nat. Mater.* **20**, 1657 (2021).
[2] K. Lin, K. Li, M. Ghorbani-Asl, et al., *J. Phys. Chem. Lett* **15**, 6010 (2024).
[3] J. Klein, T. Pham, et al., *Nat. Commun.* **13**, 5420 (2022).
[4] F. Long, M. Ghorbani-Asl, et al., *Nano Lett.* **23**, 8468 (2023).
[5] D. Kruklinskii, M. Ghorbani-Asl, et al., *Submitted* - (2026).
[6] S. Sahu, A. Hashemi, M Ghorbani-Asl, et al., *arXiv* 2601.13119 (2026).