Defect Engineering for Tuning Electronic Properties of the Janus-WSeTe

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In this study, we explore the potential of WSeTe, a Janus transition metal dichalcogenide (TMD), for novel device applications. Since TMD materials are stacked through van der Waals interactions, they lack dangling bonds on their surface, facilitating the creation of heterostructures by easily attaching another low-dimensional layer. We mainly focus on Janus TMDs which exhibit broken symmetry along the *xy* plane, potentially offering enhanced functionality compared to conventional TMDs. The unique structural properties of Janus materials lead to distinct electronic and optical characteristics[3],[4], attracting significant research interest. In this talk, we investigate the electronic properties of WSeTe, a Janus TMD, by introducing chalcogen defects to create in-gap states[4] in the insulating gap. By selectively introducing defects in either Se or Te chalcogen atoms and varying their concentration, we observe significant alterations in these defect states within the material. Employing first-principles calculations, we optimize the stable state structure and analyze the density of states and charge density to explicate the electronic tuning effects of chalcogen defects. This research provides valuable insights into utilizing WSeTe to demonstrate electronic applications through defect engineering.

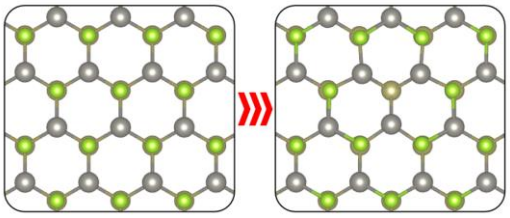

Fig.1. Monolayer WSeTe structure. the left figure is the pristine case, and the right figure is the defected case.

References

[1] T. Hu, J. Zhou, J. Dong, Y. Kawazoe, J. Appl. Phys. 116, 064301 (2014)

[2] S. You, H. Kim, N. Kim, Physica E, 144, 115400 (2022)

[3] Cong Wang, Yue-Xing Chen, Guoying Gao, Ke Xu, Hezhu Shao, Applied Surface Science, Volume 593, 153402 (2022)

[4] S. You, H. Kim, N. Kim, Current Applied Physics, **46**, 34-39 (2023)

[5] El Hamdaoui, J.; Pérez, L.M.; Ojeda-Martínez, M.; El Ouarie, N.; Díaz, P.; Laroze, D.; Feddi, E.M, Nanomaterials, **13**, 2535 (2023)

[6] Engin Torun, Fulvio Paleari, Milorad V. Milošević, Ludger Wirtz, and Cem Sevik, Nano Lett. 23, 8, 3159–3166 (2023)