Chemical doping strategy and universal small polaron formation in MoS_2

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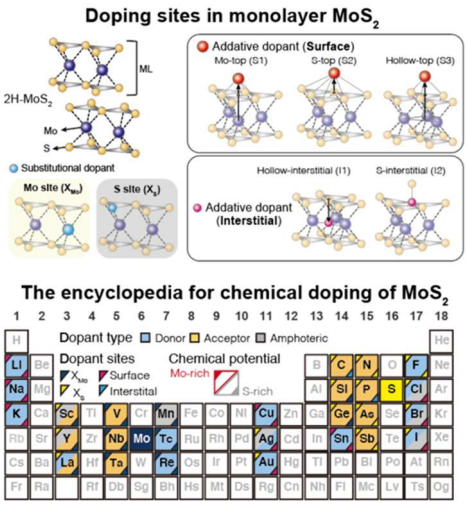
Abstract: Two-dimensional transition metal dichalcogenides (TMDs) are increasingly becoming the focus of research due to their promising applications in advanced electronics. Modifying the electrical and magnetic characteristics of TMDs via doping is crucial for enhancing the performance of TMD-based devices significantly.



Various experimental approaches to elemental doping are sought after for improving the durability and stability of TMDs. These methods enable a variety of doping configurations, encompassing substitutional dopants, surface adsorption, and lattice interstitials. In our comprehensive study, we explored the thermal stability and electrical dopability of 27 different types of acceptor and donor dopants in monolayer MoS_2, employing a self-interaction free Koopmans' compliant functional from first principles.[1] Our findings reveal universal small polaronic formations across a broad spectrum of dopants, even valid for the bulk MoS2. This implies that the impurity hopping mechanism should be predominant for electric carrier conduction in chemically doped TMDs. Our work provides a foundational theoretical background of the chemical doping of TMDs for practical applications.

References:

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2. Kim et al., "Orbital Gating Driven by Giant Stark Effect in Tunneling Phototransistors", *Adv. Mater.* **2022**, 34, 2106625.

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