When Seemingly Passive Substrates are Active

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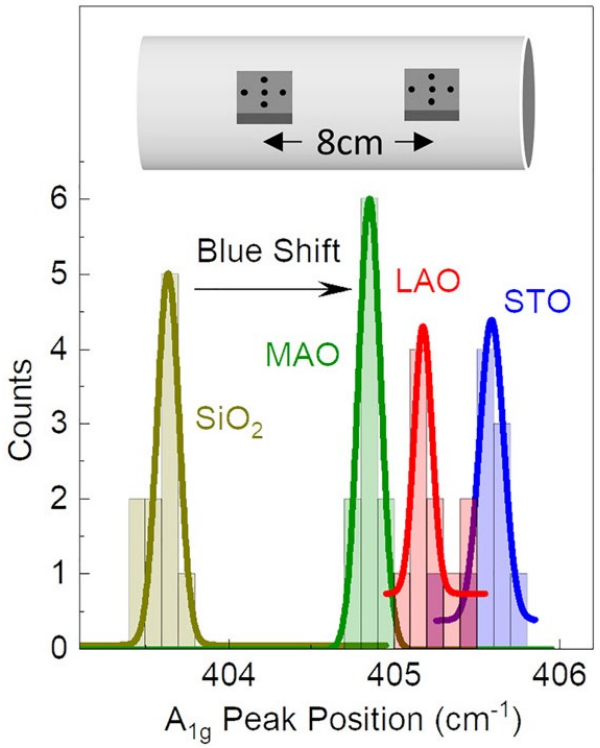
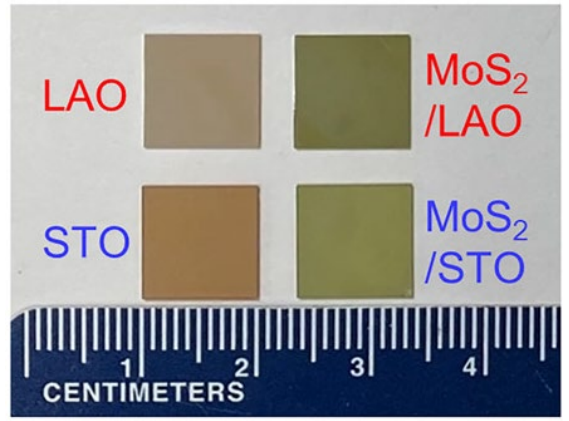
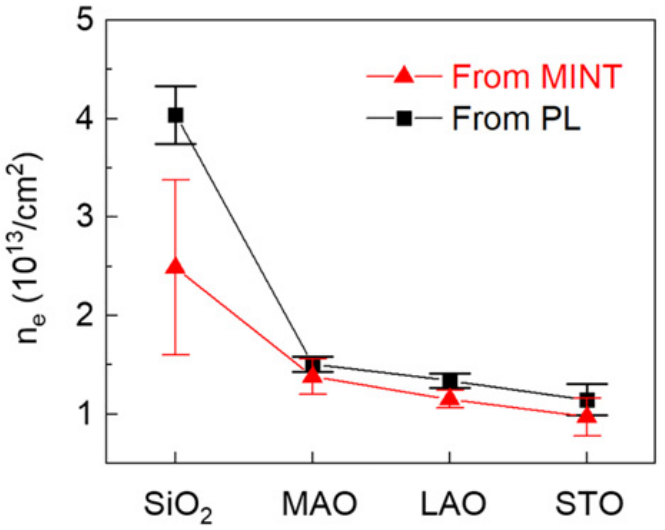
Substrates traditionally play a supporting role for the thin films grown upon them by providing purely structural support. Nonetheless for monolayer-thick transition metal dichalcogenides (TMDs), the substrate plays an active role by providing or removing charge from the TMD layer in which it is in intimate contact. The amount of charge transferred is relatively small (roughly 10^{13} electrons per square centimeter), but for monolayer-thick materials the addition or subtraction of this amount of charge can have significant doping effects on these materials, making it relevant to the operation of TMD-based electronics. Although charge transfer has been noted by prior researchers investigating TMDs, accurately predicting the charge transfer between TMDs and substrates has been out of reach.

Thanks to **PARADIM's new first-principles theory—known as mis-matched interface theory (MINT)**—this charge transfer can be accurately calculated. PARADIM's first use of MINT was to calculate the charge transfer between graphene and materials in which it was in contact; the results were in excellent agreement with experiments. Now **PARADIM's in-house team has extended these calculations to TMDs** and performed experiments to test the calculations by growing films of the TMD MoS_2 on several oxide substrates including SiO_2, $MgAl_2O_4$, $LaAlO_3$, and $SrTiO_3$. The measured charge transfer is found to be in excellent agreement with the predictions of MINT. The ability to employ a substrate to quantitatively and reproducibly control the doping of a TMD film grown upon it is a powerful addition to the traditional means of controlling the doping through electrostatic gating or the addition of chemical impurities.







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