Surface susceptibility and conductivity of monolayer-MoS_2 & -WSe_2

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In the post graphene era, monolayer transition metal dichalcogenides (TMDs) are well documented among all the 2D materials.[1-3] Owing to the quantum confinement effects in the monolayer limit, they shown favorable electronic properties. However, accurate modelling of electronic properties of TMDs is not trivial. This work targets a quantitative agreement between first principle studies and ellipsometric experimental results.

To compute the surface susceptibility and optical conductivity of monolayer MoS_2 and WSe_2, a recent formulation for the optical properties of 2D crystals from first principle studies[4, 5] has been employed (spin-orbit and excitonic inclusive). The main features (A, B, C, D peaks) of the computed spectra are clearly resolved also in ellipsommetry measurements, whilst theoretically we also observe the emergence peaks that can be attributed to excited exciton states, which is also observed in the second-derivative ellipsometry results. Many of these excited states were never reported in the ellipsometric measurements at ambient conditions, thus, these results demonstrate the importance of merging computational and experimental methods to characterize the optical response of 2D crystals as well as highlighting the high degree of precision that ellipsometry can reach in measuring both surface susceptibility and optical conductivity.

References

[1] Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman, and M.S. Strano, Nat. Nanotechnol., 7 (2016) 699.
[2] D. Jariwala, V. K. Sangwan, L. J. Lauhon, T. J. Marks, and M. C. Hersam, ACS Nano, 8 (2014) 1102.
[3] S. Manzeli, D. Ovchinnikov, D. Padauier, O. V. Yazyey, and A. Kis, Nat. Rev. Mater., 2 (2017) 17033.
[4] L. Matthes, O. Pulci, and F. Bechstedt, Phys. Rev. B, 94 (2016) 205408.
[5] L. Matthes, O. Pulci, and F. Bechstedt, New J. Phys., 16 (2014) 105007.

Figures

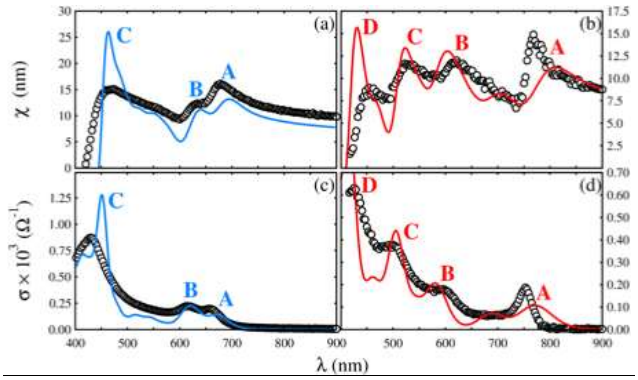

Figure 1: Comparison of the calculated (lines) and experimental (circles) surface susceptibilities of monolayer (a) MoS_2 and (b) WSe_2 and optical conductivity of monolayer (c) MoS_2 and (d) WSe_2.