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# WanTiBEXOS: a Wannier based Tight Binding code for excitonic and optoelectronic properties of solids

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## Abstract

The GW plus the Bethe-Salpeter (BSE) equation approach becomes a methodology commonly used for computing the quasiparticle and optical properties of condensed-matter systems. However, GW approach requires a fine k-point sampling of the Brillouin zone, and GW plus BSE (GW-BSE) demands an even finer k-point sampling. Hence it is rather easy to reach the limits of what can be practically computed. In order to overcome this challenge, we have developed WanTiBEXOS, a parallel computational FORTRAN code, constituted of an effective tight-binding (TB) model in conjunction with BSE framework. The former is constructed by means of maximally localized Wannier functions. The WanTiBEXOS package can be executed via any density functional theory package interfaced with Wannier90 code[1] with computational time being reduced up to one or more orders of magnitude in comparison with that of GW-BSE. In order to demonstrate its the reliability, flexibility, efficiency and versatility of WanTiBEXOS, we provide the input files to perform electronic and optical property calculations for the representative materials, including conventional bulk semiconductors, $CsGeCl_3$ super cubic,[2] nano-monolayer materials and van der Waals heterostructures. The results are also presented accordingly.

## References

[1] Mostofi et. al., Computer Physics Communications 178(9), 685 (2008)
[2] A. C. Dias et. al., Journal of Physical Chemistry C 125(35), 19142 (2021)

## Figures

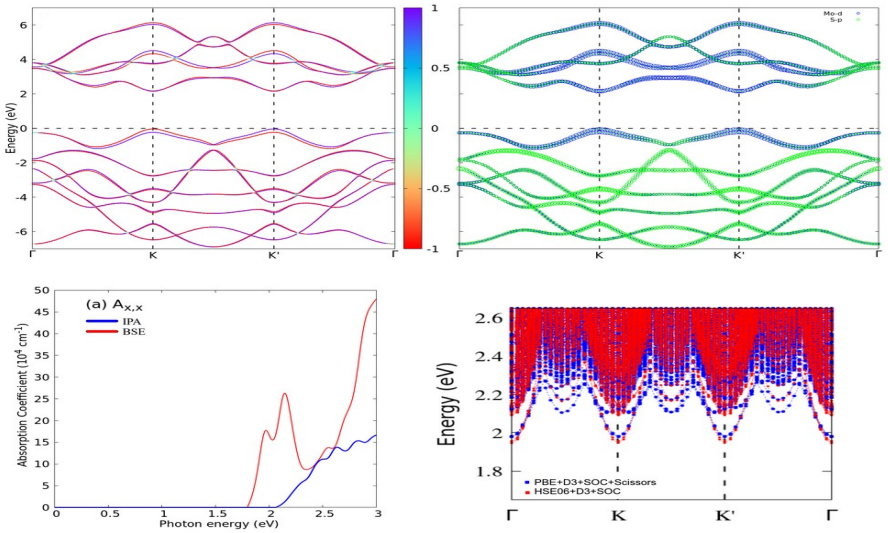


**Figure 1:** WanTiBEXOS features demonstration: upper pannel – projected band structure (spin and atomic species contribution), lower pannel – Absorption coefficient at IPA and BSE levels and Exciton band structure with PBE+SCS and HSE06 XC functionals.