# Quantum/classical method for dielectric properties of layered 2D materials

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Van der Waals heterostructures (vdWHs) hold great promise for technological applications by merging the unique properties of 2D materials with extensive design flexibility. However, theoretical modeling of these structures is challenging. We introduce a new mixed quantum/classical model taking outset in the Quantum Electrostatic Heterostructure (QEH) model[1,2], which offers an efficient and accurate description of the dielectric properties of vdWHs. For representing the induced densities and potentials, we use a hierarchical basis of dielectric eigenstates of the isolated monolayers. We showcase the model by computing exciton binding energies and out-of-plane screening for a select set of vdWHs containing TMDs and Janus monolayers.

## References

[1] Andersen, K., Latini, S., & Thygesen, K.S. *Nano letters* 15.7 (2015): 4616-4621.
[2] Gjerding, M. N., Cavalcante, L. S. R., Chaves, A., & Thygesen, K. S. *The Journal of Physical Chemistry C* 124.21 (2020): 11609-11616.
[3] Latini, S., Olsen, T., & Thygesen, K. S. *Physical Review B*, *92.24* (2015): 245123.
[4] H.-P. Komsa and A. V. Krasheninnikov, *Physical Review B, 86* (2012): 241201.

## Figures

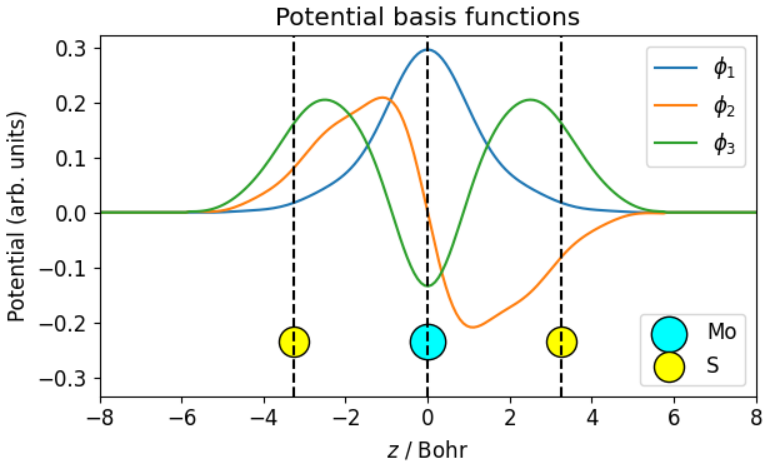


**Figure 1:** The dielectric response of each layer in the vdWH is described in a finite basis consisting of eigenfunctions of the monolayer dielectric function. This set describes the most important screening channels using the smallest possible number of basis functions.