Progressive cluster approach to photoemission in transition metal dichalcogenides

M. J. Ambrosio, E. Plesiat, P. Decleva, P.M. Echenique, R. Díez Muiño and F. Martín

Universidad Autónoma de Madrid, Avda. F. Tomás y Valiente 7, Madrid, Spain
mj.ambrosio@dipc.org

We present a fully atomistic approach to transition metal dichalcogenides (TMDC) angle-resolved core-level photoemission[1,2]. We calculate the fully differential cross section and Wigner time delay from the dipole-transition elements. The initial- and final-state wavefunctions are generated via a central partial-wave expansion complemented by smaller off-center auxiliary partial-wave expansions that approach B-Spline methodology [3]. Electrostatic interactions between the active electron and the rest of the cluster are taken into account through a DFT model with a LB49 exchange-correlation potential.

By comparing the cross sections and Wigner delays obtained for different model clusters we are able to dissect the underlying processes taking place as the photoelectron scatters throughout its parent system. This gradual-construction approach from smallest to largest cluster provides a reference to indicate which neighboring atoms the photoelectron is deflecting off of.

Figure 1 (left) ilustrates how we construct the clusters by adding atom perimeters respecting the group symmetry, D3h and C3v in our study cases. As an example we show the resulting WSe_2 W*4f* photoemission cross sections (middle) from model cluster W_7Se_6 and Wigner time delays (right), which will be compared to the corresponding parts from smaller or larger clusters.

References

[1] M. J. Ambrosio *et al.*, J. Phys. B, 105 (2022) 125405
[2] M. J. Ambrosio *et al.* , Chem. Phys., 577, (2022) 111476
[3] M. Venuti et al., Chem. Phys., 234 (1998) 95

Figures