## Quantum Stereodynamics of cold collisions between two aligned molecules

Thursday 7 September 2023 17:10 (25 minutes)

One of the most fundamental questions in molecular dynamics is the dependence of a collision outcome on the relative orientation/alignment of the reactants, i. e. the stereodynamics of a collision process. For bimolecular gas phase reactions, it is possible to address this question by polarizing the reactants bond-axis and/or rotational angular momentum.[1-4]

Here, we will illustrate how the outcome of a collision can be controlled by selecting the relative geometry of the colliding partners before they start to interact. In particular, we will focus on the collisions at low energies, which proceed with contributions from just a few partial waves, such as those between two aligned D2 molecules, whose angular distributions have been measured recently by Zhou et al. [2]. Our results based on full-dimensional coupled-channel scattering calculations reveal that the experimental angular distribution is caused by a L=4 resonance, and that key features of the experimental angular distributions are only captured when four-vector correlations in aligned-aligned molecular collisions are accounted for.

## References

[1] T. R. Sharples, J. Leng, T. F. M. Luxford, K. G. McKendrick, P. G. Jambrina, F. J. Aoiz, D. W. Chandler and M. L. Costen. Nat. Chem., 10, 1148 (2018)

[2] H. Zhou, W. E. Perreault, N. Mukherjee, and R. N. Zare, Nat. Chem. 14, 658 (2022).

[3] W. E. Perreault, N. Mukherjee, and R. N. Zare, Science 358, 356 (2017).

[4] P. G. Jambrina, J. F. E. Croft, J. Zuo, H. Guo, N. Balakrishnan, and F. J. Aoiz. Phys. Rev. Lett. 130, 033002 (2023)

Author: GARCÍA JAMBRINA, PABLO (Universidad de Salamanca)

Presenter: GARCÍA JAMBRINA, PABLO (Universidad de Salamanca)

Session Classification: Invited talks