Dissociative Electron Attachment to Polyatomic Molecules: *Ab initio* Calculation of Attachment Amplitudes and Nonadiabatic Dissociation Dynamics

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Although dissociative electron attachment (DEA) through metastable anion resonances has been studied experimentally and theoretically since the 1960s [1], it can be said that the field has undergone a renaissance since the introduction of the techniques of momentum imaging [2] and velocity-slice imaging in DEA experiments [3,4]. These experiments provide a degree of insight into the dissociative attachment process not previously accessible. However, without the observation of the final momenta of at least two fragments (the anion and a neutral fragment), it is not possible to directly connect these measurements to the body frame dynamics of DEA. For that reason a combination of the theoretical calculation of attachment amplitudes (Fig. 1) and the experimental measurement of the angular dependence of the anion fragment, has been necessary for the detailed interpretation of this new generation of experiments.

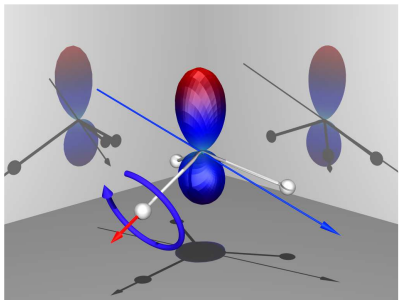

Fig. 1 Entrance amplitude for the $^2A_1$ Feshbach resonance in NH_3

We will discuss the calculation of attachment amplitudes that give the probability for resonant electron attachment to the neutral molecule as a function of the incident electron momentum in the body frame. Thus far, the determination of attachment amplitudes has only been possible in full electron-scattering scattering calculations. The attachment amplitude is not enough to identify the dynamical pathway of dissociation in many cases. Conical intersections between anion potential surfaces are more the rule than the exception, and they can also have features that negate direct dissociation consistent with "axial recoil" dynamics. We will illustrate these phenomena with a complete analysis of DEA to ammonia via the $^2A_1$ Feshbach resonance at 5.5 eV, which produces anion products exclusively via nonadiabatic nuclear dynamics, and with preliminary results on DEA to formic acid, which may be more complicated still.

References

[1] I I Fabrikant, S Eden, N J Mason and J Fedor, "Recent Progress in Dissociative Elecron Attachment: From Diatomics to Biomolecules, Adv. At. Mol. Opt. Phys. **66** 545 (2017).
[2] D S Slaughter, A Belkacem, C W McCurdy, T N Rescigno and D J Haxton, "Ion-momentum imaging of dissociative attachment of electrons to molecules," *Journal of Physics B: Atomic, Molecular and Optical Physics*, **49**, (2016), 222001.
[3] B Wu, L Xia, H K Li, X J Zeng and T S Xi, "Positive/negative ion velocity mapping apparatus for electron-molecule reactions," *Rev. Sci. Instrum.*, **83**, (2012), 013108.
[4] E Krishnakumar, V S Prabhudesai and N J Mason, "Symmetry breaking by quantum coherence in single electron attachment,"*Nature Physics*, **14**, (2018), 149-153.