Attosecond charge migration in $HCCI^+$ and its coupling to nuclear motions

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Recently, quasi-field-free charge migration in $HCCI^+$ was investigated.[1] Experimentally, the initial state (t = 0) is reconstructed as superposition of the electronic ground and first excited states. This initial state can be prepared by ultrafast ionization of HCCI [1] or by electronic excitation of $HCCI^+$.[2] The excess electronic charge then migrates periodically between the acetylenic and ionic moieties, with period τ = 1.85 fs. The maximum axial electronic flux occurs between the two moieties where the axial density has its local minimum; the electronic flux is launched already during the laser pulse that prepares the initial state; it is possible to optimize the electronic flux.[1-3]

Adding effects of nuclear motions, the above coherent charge migration model needs to be improved.[4] An apparent effect is the decoherence of charge migration – by analogy, this causes the emergence of the classical world from quantum states. The effect of decoherence in $HCCI^+$ can already be large after a few periods of charge migration. In addition I discover a new phenomenon, the revival or partial revival of charge migration. This is due to (partial) recurrences of the overlap of the nuclear wave packets in the electronic ground and excited states.

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[3] H. Ding, D. Jia, J. Manz, Y. Yang, Mol. Phys., 2017, **115**, 1813.
[4] D. Jia, J. Manz, Y. Yang, in preparation.