Laser control of the photodissociation of CO^{2+}

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The combination of electronic structure calculations by quantum chemistry techniques with wave packet propagation methods provides a powerful way to study reactive processes at a fully quantal level. This approach has been used with success to study charge transfer, photodissociation, or radiative association processes [1-3]. One of its advantages is the possibility to include an electromagnetic field into the dynamics, allowing the control of the outcome of reactions, for example using optimal or local control algorithms. Here we illustrate these methods on the photodissociation of the carbon monoxide dication CO^{2+} into a specific channel. In particular, we show the efficiency of the local control algorithm to find a simple pulse despite the complex nonadiabatic dynamics [4]. This molecular ion also provides an interesting example as it can be produced experimentally in a single vibrational state.

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References

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