

Steve Ndengué, Richard Dawes

Missouri University of Science and Technology, Rolla, USA

The Heidelberg MCTDH package is an important multi-tasking toolbox useful for various applications of quantum dynamics to fields like astrochemistry and atmospheric chemistry.

In our talk, we will show some of our recent investigations using principally the MCTDH code.

We will present for example the ozone spectroscopy and photodissociation related to the ozone isotopic anomaly, the H+CO inelastic scattering with inclusion of the Renner-Teller coupling, or a recent calculation of the H₂O+Ar inelastic scattering.

We will also discuss the potential limitations and advantages of the code and mention some ongoing investigations.