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Time-dependent quantum defect theory for dissociative recombination of diatomic molecules¹ SAMANTHA SANTOS, VIATCHESLAV KOKOOULINE, Physics department of University of Central Florida, CHRIS GREENE, JILA, University of Colorado at Boulder — Dissociative recombination (DR) of molecular ions with electrons takes place on atomic quantum dynamics level with the incoming electron being captured by the field of a molecular cation transferring its energy to the nuclear motion. In its descending route, the electron goes through a series of Rydberg states until the vibration of the nuclei couples one of these resonances to a pre-dissociative state of the molecule. The DR process ends with the fragmentation of the molecule. Most studies on DR have been conducted with different diatomic or triatomic molecular ions in the time-independent framework of multi-channel quantum defect theory (MQDT). The present work uses MQDT to monitor time-dependent evolution of the DR process. The obtained results provides time-dependent picture of how a localized wave packet of incoming electrons transfers its energy to the vibration of the molecule through the Rydberg states. The wave packet is partially reflected back to the ionization channel. A model diatomic system has been used so far, and vibrational dynamics is described by Siegert pseudo-states.

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