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Recent developments in theoretical treatment of dissociative recombination[1] VIATCHESLAV KOKOOULINE, University of Central Florida, NICOLAS DOUGUET, SAMANTHA FONSECA DOS SANTOS, ANN OREL, University of California at Davis — Over last few years, we have been developing a theoretical treatment of dissociative recombination (DR), which can be general and simple enough to be applied to a wide range of small polyatomic ions. In this work we present such a approach, which is based on the first principles only. It relies on the scattering matrix calculations for electron-ion collisions performed for fixed nuclei for a number of geometries near the equilibrium position of the ion. The obtained geometry-dependent scattering matrix is then used to calculate the cross section for electron capture into a Rydberg state of an excited vibrational mode of the molecule. This is made by a standard vibrational frame transformation from the molecular to laboratory frame. Assuming that the autoionization of such Rydberg states is much slower than predissociation, the electron capture cross section gives approximately the DR cross section. We will give two examples of such DR calculations, for the HCO^+, N_2H^+ ions. The obtained theoretical DR cross sections agree well with available experimental results.

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Viatcheslav Kokoouline
University of Central Florida

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