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Analytical formulation for potential energy surfaces in molecular collision dynamics of cold plasma FELIX IACOB, Faculty of Physics, West University of Timioara, Romania, NICOLINA POP, Department of Fundamental of Physics for Engineers, Politehnica University of Timisoara, Romania — We consider the characteristic discharge chemistry processes in cold plasma, which are mainly driven by free electrons, but also by ion-molecule reactions. In order to obtain a better description of the collision between two molecules, a form for the molecular interaction potential should be assumed. Determining theoretically the rate coefficients, first one has to focus on electronic calculations of potential energy surfaces (PES), in BO approximation, further used to study the motion of the nuclei (collision dynamics). Currently used are ab-initio models, in this work an analytical expression of potential energy surface is derived and used to describe the molecular dynamics in cold plasmas. A specially attention was given to the exotic cases where the present data fully support a model that assumes potential barriers or bottle necks. Some dissociative recombination cross section where calculated using this new analytical form in the case of electron reacting with HD+. Also the Maxwell-Boltzmann rates have been calculated being of particular interest to the plasma research. The result are compared with literature. Low temperature experiments have shown that there can be significant deviations from such simple models.

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