Charge transfer in Sodium Iodide collisions

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Sodium Iodide (NaI) have over the years served as a prototype system in the studies of avoided crossing dynamics. Here, the charge transfer collision reactions $Na+I \leftrightarrows Na^{+}+I^{-}$ (mutual neutralization and ion-pair formation) are studied from an *ab initio* approach and the total- and differential cross sections are calculated for the reactions. This involves electronic structure calculations on NaI to obtain adiabatic potential energy curves, nonadiabatic coupling and spin-orbit coupling followed by nuclear dynamics, treated fully quantum mechanically in a strict diabatic representation. A semi-empirical spin-orbit coupling model is also investigated and the effects of rotational coupling is estimated. The calculated total- and differential cross sections are compared with measured ion-pair formation cross sections and analysed via the semi-classical Landau-Zener model.