

## AB INITIO STUDY OF ION-PAIR STATES OF THE IODINE MOLECULE

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Ion-pair states of the  $I_2$  molecule have been the subject of many experimental studies and to date all 18 states correlating with  $I^+(^3P_{J=2,1,0}, ^1D_2) + I^-(^1S_0)$  asymptotes are known from experiment. This contribution reports on *ab initio* study of the  $I_2$  molecule with an emphasis on the ion-pair states. Figure shows experimental and calculated potentials of the ion-pair states correlating with  $I^+(^3P_2) + I^-(^1S_0)$  asymptote (energy is relative to  $I(^2P_{3/2}) + I(^2P_{3/2})$  asymptote).

