Electron capture in collisions of C V with molecular hydrogen

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Carbon as a plasma facing component important for fuel retention and recycling is a practically relevant edge plasma impurity in all of its charge states. A theoretical study of electron capture probabilities is reported for the C^{4+}/H_2 system using a large manifold of electronic states in the collisional configuration corresponding to the planar symmetric impact, which efficiently favors electron capture in terms of the initial electron density on the molecular hydrogen as exposed to the projectile. The potential energy curves are obtained with the multi-reference single- and double-excitation configuration interaction method implemented in the program code of Wuppertal group. In the singlet A_1 symmetry thirty five roots were needed to compute the initial state configuration of this exothermic process. The potential energy surface section is obtained with 464 points in varied separation of the hydrogen centers. The single and double electron capture cross sections obtained in experiments [1,2] are known to vary rather slowly with collision energy consistent with multi-route transition regime dynamics. Therefore the present theoretical treatment focuses on the comparison of several diabatic coupling extraction schemes to obtain approximate bounds on the accuracy of such cross section estimates. Our present procedure reasonably compares with the experimental data available in the literature (NIFS CHART database), and may add to data production efforts for quantitative understanding of fusion edge plasma processes [3].

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