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Workshops

Theoretical and Computational Studies of Non-Equilibrium and Non-Statistical Dynamics in Gas-Phase, Condensed-Phase, and Interfacial Reactions

April 11, 2016 to April 13, 2016
Location : CECAM-FR-IDF, Institut Heny Poincaré (salle 314), Paris, France

Details   Participants   Program   Posters   Abstracts

Quassi-Classical Results of Reactions Involving the Formation and Transformation of H3+

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Abstract

Quasi-Classical studies of the H3+ formation reaction[1]
H2 + H+ --> H + H3+
and the exchange reaction[2]
H2+H3+ --> H3+ + H2
will be presented, on full dimensional potential energy surfaces[3,4]. In the first case, the non-adiabatic effects are studied using the Molecular Dynamics with Quantum Transitions[5] as a function of the translational energy and vibrational excitation of H2+.

In the H5+ system, the statistical approach of Park and Light[6] is extended by performing quassiclassical trajectories, including an approximate method to account for the zero point energy[2], to calculate the identity/hop/exchange probabilities. This allows to describe the transition between full scrambling statistical behavior, characteristic at low temperatures, and a more direct hop mechanism at higher temperatures.

Comparison with experimental results[7,8] will be also discussed.

References

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