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Cold and Ultracold Chemistry with Charged and Neutral Particles

Different chemical reactions at very low collision energies between ions and neutrals are investigated from a quantum chemistry perspective. In particular, three-body processes, i.e., molecular formation from three free atoms $(A + A + A- > A_2 + A)$, and atom-molecule charge transfer mechanism $(A_2^+ + A- > A_2 + A^+)$. The presence of ion-neutral interactions establishes a different threshold for cold and ultracold collisions, leading to the influence of many partial waves at 1mK of collision energy for Rb, for instance. This peculiarity of the systems at hand complicates the task to perform quantum calculations, however a classical trajectory method will be suitable for the simulation of such chemical processes. A very recent classical trajectory calculation method [1] will be employed for the calculations of the rate constants for different chemical reactions present in hybrid traps experiments [2] and in Bose-Einstein condensates ones [3].
[1] J. Pérez-Ríos, S. Ragole, J. Wang and Chris. H. Greene, J. Chem. Phys. 140, 044307 (2014). [2] A. Härter, A. Krükow, W. Schnitzler, S. Schmid and J. HeckerDenschlag, Phys. Rev. Lett. 109, 12301 (2012). [3] J. B. Balewski, A. T. Krupp, A. Gaj, D. Peter, H. P. Büchler, R. Löw, S. Hofferbeth and T. Pfau, Nature 502, 664 (2013).

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