Stereodynamic and Non-adiabatic Effects in Cold and Ultracold Collisions

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The prospect of probing chemical reactions in the extreme quantum limit has become a reality in recent years thanks to the rapid advancement in molecule cooling, trapping, and imaging technologies for quantum state-resolved product detection [1,2]. Ultracold molecules also offer exciting opportunities to explore electronically non-adiabatic effects in chemical reactions that are resolved at the single partial-wave level [3]. Figure 1 illustrates large non-adiabatic effect in the ultracold limit in the rotationally resolved rate coefficients for the Li+LiNa→Li_2+Na chemical reaction [3]. Here the non-adiabatic effect arises from constructive quantum interference due to a conical intersection between the ground and an excited electronic states that are accessible in the ultracold limit. Stereodynamic control of inelastic rotational quenching in bimolecular collisions has also been demonstrated recently using the Stark-induced Adiabatic Raman Passage (SARP) technique where isolated resonances control the product angular distribution [4]. I will discuss recent progress in the theoretical treatment of the Li+CaF→LiF+Ca chemical reaction in the cold regime as well as non-adiabatic dynamics in the ultracold Li+LiNa→Li_2+Na reaction [3]. I will also discuss stereodynamic control of bimolecular collisions involving HD and D_2 prepared by the SARP techniques [4,5].

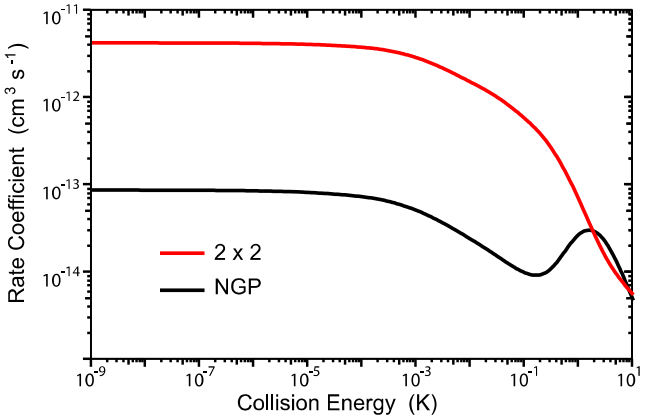

Figure 1: *Rotationally resolved rate coefficients for the Li + LiNa(v = 0, j = 0) → Li_2(v' = 3,j' = 5) + Na reaction as a function of collision energy. The red and black curves are the rates computed using the coupled two-state diabatic (2×2) and single surface adiabatic (NGP) methods, respectively. The geometric phase (GP) which is included in the diabatic 2×2 calculations gives rise to constructive quantum interference and a significantly enhanced ultracold rate coefficient relative to the NGP calculation which ignores the GP.*

Index Terms: ultracold collisions, non-adiabatic effects, stereodynamic control, ultracold chemistry.

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