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Ultracold chemistry and dynamics of Li+CaF collisions¹ MASATO MORITA, Univ of Nevada - Las Vegas, QIAN YAO, CHANGJIAN XIE, HUA GUO, University of New Mexico, BRIAN K. KENDRICK, Los Alamos National Laboratory, N. BALAKRISHNAN, Univ of Nevada - Las Vegas — Ultracold polar molecules are actively being explored as potential candidates for quantum simulation, quantum information processing, and precision testing of fundamental physics. Polar molecules involving alkaline earth atoms such as CaF have attracted considerable attention and direct laser cooling and trapping of CaF have recently been reported. A second-stage cooling may involve sympathetic collisions with ultracold alkali metal atoms such as Li but its applicability may be limited by exothermic reactive scattering. Here we explore elastic and inelastic (reactive) collisions of Li with CaF molecules in the cold and ultracold regime. In particular, we report the characteristics of highly anisotropic potential energy surface of Li+CaF and LiF+Ca obtained from extensive ab initio calculations and quantum scattering calculations of the ultracold Li+CaF → LiF+Ca chemical reaction using hyperspherical coordinates.

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