THE HARPOON REACTION Li_2 + F AND ULTRACOLD CHEMISTRY

K. WRIGHT and I. C. LANE, *School of Chemistry and Chemical Engineering, Queen's University of Belfast, Belfast, BT9 5AG*.

A new set of potential energy surfaces have been calculated for the classic harpoon reaction Li_2+ F to model s-wave reactive scattering at ultracold temperatures. This reaction type has a number of advantages for the experimental study of ultracold reactions namely 1) a large reaction cross-section, 2) the absence of significant barriers to reaction and 3) the ability to create quantum state selected Li_2 molecules by magnetic resonances in ultracold traps. In addition, the molecular product LiF has a very strong permanent dipole and is consequently a possible candidate for a molecular qubit. Multi-reference $ab-initio$ calculations are shown to correctly describe the interaction between ionic and covalent surfaces, and the validity of the simple harpoon model is explored.