

THE HARPOON REACTION $\text{Li}_2 + \text{F}$ AND ULTRACOLD CHEMISTRY

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A new set of potential energy surfaces have been calculated for the classic harpoon reaction $\text{Li}_2 + \text{F}$ 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.