Potential energy $1^2A'$ surface of the Li_2+Li doublet ground state

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With the success of ultracold molecular formation among the alkali metals over the last few years, the dynamics of molecules in an ultracold trap have become an important topic of interest to many physicists. Both heteronuclear and homonuclear lithium diatoms have been formed in the ground electronic state with great success using combinations of photoassociation and Feshbach resonances. A precise potential energy surface of the ground lithium trimer in the doublet state, $Li_2[X^1\Sigma_g^+]$+Li$[^2S]$ for the atom-diatom collision problem has been calculated here for use in reaction scattering calculations for the prediction of ultracold trimer formation.

The $1^2A'$ surface was calculated using the Stevens-Basch-Krauss (SBK) [J. Chem. Phys. 81, 6026 (1984)] effective core potential with a core polarization potential and augmented SBK basis set at the full configuration interaction level. Using the Labello *et al* [Int. J. Quant. Chem. 106, 3140 (2006)] augmented SBK basis set, we optimized the disassociation energy of the $Li_2[X^1\Sigma_g^+]$ ground state at the full configuration interaction level with the SBK effective core potential with core polarization. Ground and excited potential curves are also calculated for C_{2v} symmetry at second order spin restricted open-shell Møller-Plesset perturbation theory and CASSCF level, where a conical intersection is shown to occur between the 1^2A_1 and 1^2B_1 surfaces near the trimer equilibrium geometry.