

Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

***Ab initio* potential energy surfaces $1^4A'$, $2^4A'$, $1^4A''$ and $2^4A''$ of Li_3 in a constant external magnetic field** JUAN BLANDON, University of Oklahoma, XUAN LI, University of British Columbia, DANIEL BRUE, GREGORY PARKER, University of Oklahoma — Molecular potential energy surfaces (PESs) have played an essential role in understanding the field-induced interactions in atomic/molecular systems. External magnetic fields are relevant because they are used to control the pairwise interactions in atomic quantum gases. We present accurate PESs for three fermionic ^6Li atoms under a constant external magnetic field. Calculations are made using the diatomics-in-molecules method [1], accounting for fine and hyperfine interactions. PESs are constructed using full configuration interaction for the three valence electrons, and a global-fit method [2] is used to obtain the three-body terms. These PESs can be used, for example, to study three-body recombination near overlapping Feshbach resonances.

[1] J. C. Tully, J. Chem. Phys. **58**, 1396 (1973)

[2] A. Aguado *et al.*, Comput. Phys. Commun. **108**, 259 (1998)

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Date submitted: 26 Jan 2010

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