Abstract Submitted
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Ground state of lithium: evidence from the de Haas-van Alphen effect analysis[1] SABRI ELATRESH, Department of Chemistry and Chemical Biology, Cornell University, Baker Laboratory, Ithaca, New York 14853-1301, WEIZHAO CAI, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, NEIL ASHCROFT, Laboratory of Atomic and Solid State Physics, Cornell University, Clark Hall, Ithaca, New York 14853-2501, ROALD HOFFMANN, Department of Chemistry and Chemical Biology, Cornell University, Baker Laboratory, Ithaca, New York 14853-1301, SHANTI DEEMYAD, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, STANIMIR BONEV, Lawrence Livermore National Laboratory, Livermore, California 94550 — The lithium Fermi surface in the bcc, fcc, hcp, and 9R structures is computed at zero pressure and temperature using first principles theory. It is shown that measurements of the Fermi surface based on the de Haas-van Alphen effect can be used as a diagnostic method to investigate the low temperature phase diagram of lithium. The theoretical results are presented in conjunction with experimental data, which could allow us to rule out some of the phases as the ground state structure of lithium at zero pressure.

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