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Dipole moments of ultra-cold polar molecules: a quantum Monte Carlo study MICHAL BAJDICH, SHI GUO, LUBOS MITAS, CHiPS, Department of Physics, NCSU, Raleigh, NC, PETER J. REYNOLDS, Physics Division and Physical Sciences Directorate, U.S. ARO, Durham, NC — Recently, there has been a great deal of interest in the production of ultra-cold heteronuclear molecules having large electric dipole moments [1]. This is of interest both for fundamental reasons as well as for applications such as qubits for quantum computing [2]. In this work, we calculate the dipole moment of a potentially implementable two-atom alkaline-alkaline-earth molecule, LiSr. We use correlated wave-function methods including both the quantum chemical configuration interaction (CI) method, and a stochastic quantum Monte Carlo (QMC), to calculate the potential energy surface and dipole moment. We study the dipole moment with increasing accuracy of correlated wave-functions. We then variationally re-optimize the wave-functions, which then serve as the representation of the Fermion nodes in the fixed-node QMC. To treat the Sr atom we employ two types of effective core potentials (ECPs), large core ECPs have only s -states in the valence space, while the small core ECP's valence space includes also the highest s and p semi-core sub-shells. We find significant sensitivity of the dipole moment on both the size of the valence space and on the accuracy of the Fermion nodes. [1] B. Damski, *et. al* Phys. Rev. Lett. 90, 110401 (2003). [2] D. DeMille, Phys. Rev. Lett. 88, 067901 (2002).

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