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Fixed-Node Errors in Diffusion Monte Carlo Study of Li Molecular and Solid Systems KEVIN RASCH, LUBOS MITAS, North Carolina State University — We study the fixed-node bias in the Diffusion Monte Carlo calculations of Li systems such as Li dimer, Li clusters, and Li body-centered cubic crystal at the equilibrium lattice constant. The calculations include both core and valence electrons in order to avoid any possible impact by pseudopotentials. We examine the fixed-node errors for different types of orbitals and wave-function forms. We use estimations of exact total energies from alternative approaches such as correlated basis set methods or from experiment. The results suggest that for Li systems it is possible to construct accurate wave-functions which recover correlation energy at 97-99 % of correlation energy in the full many-body framework.

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