Abstract Submitted
for the GEC11 Meeting of
The American Physical Society

Interaction between LiH and Li based on electronic structure calculations YIMING MI, Graduate Department, Shanghai University of Engineering Science, XINGXING ZHAO, School of Fundamental Studies, Shanghai Univ. of Engineering Science, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo — The potential energy surface for the LiH molecule interacting with the Li atom with adiabatic approximation was calculated in terms of ab initio methods. The interaction potential was obtained by using a combination of the explicitly correlated unrestricted coupled-cluster method with single, double, and noniterative triple excitations for the core-core and core- valence correlation and full configuration interaction for the valence-valence correlation. A global minimum has acquired for the potential energy surface under the condition of fixing the Li-H bond length at the monomer equilibrium distance. And a strongly anisotropic potential of the ground state of Li-LiH is obtained too. The interaction between the two potential energy surfaces and its possible impact on the collisional dynamics are also analyzed in this work.

Yiming Mi
Graduate Department, Shanghai University of Engineering Science

Date submitted: 22 Jul 2011 Electronic form version 1.4