
Quantum mechanical calculations on the excited states of the Li₂F molecule

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Résumé

The lowest electronic states of alkali metal cluster with adatoms and admolecules have different electronic distribution, leading to diverse ionicities between the substrate and the adsorbate, among the states. In addition, these systems may serve as a prototype for covalent-ionic system, where coupling between various states leads to barrierless adsorption and hence subsequently finds extensive applications in the ultracold regime. Accurate quantum calculation on these systems would provide valuable insights into the scattering resonances between the metallic surface and the overlying gaseous adsorbate. One of the excellent candidate of covalent-ionic system is obtained when a fluorine atom (F) with a very high electron affinity (3.4 eV) approach a loosely ionizable (5.1 eV) lithium dimer (Li₂). Our main goal is to unfold the collision process, which would involve contribution from ground and lower lying excited states. We have calculated five low-lying 2A₁ states, using multireference ab initio methods, by constraining the F atom to approach the center of mass of Li₂ perpendicularly, so that whole scattering process could be resolved into C_{2v} symmetry. The potential energy curve of this interaction reveals a barrierless collisional cross-section for the ground state and multiple avoided crossings at rather large distances between the excited states. A dipole moment analysis of the ground state shows that it is not as ionic as expected.

Mots-Clés: alkali clusters, covalent, ionic systems, excited states, potential energy surfaces, multireference methods

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