

Abstract Submitted  
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**Electronic Transition Dipole Moment and Radiative Lifetime Calculations of Lithium Dimer Ion-Pair States** AYDIN SANLI, DAVID BEECHER, MARJATTA LYYRA, Temple University, SYLVIE MAGNIER, Université des Sciences et Technologies de Lille, France, ERGIN AHMED, Temple University — Lithium dimer molecular electronic states exhibit double wells and shoulders due to the interaction with the  $\text{Li}^+ + \text{Li}^-$  ion-pair configuration. The double well behavior is predominantly observed for higher lying electronic states of  $^1\Sigma_g^+$  symmetry at larger internuclear distance. The ion-pair character of these potential energy curves makes their lifetimes also interesting because of the unusual behavior of their transition dipole moments which exhibit rapid changes around potential curve shoulders and double wells. In this work we present a computational study of lifetimes and transition dipole moment matrix elements for the lithium dimer ion-pair states. We report here the *ab initio* calculated electronic transition dipole moments between the  $n^1\Sigma_g^+$  states and the  $A^1\Sigma_u^+$  state, that vary strongly as a function of internuclear distance. In addition, we have calculated the radiative lifetimes,  $\tau$ , of these ion-pair states and compare them with experimental results from literature when available.

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