Electronic Transition Dipole Moment and Radiative Lifetime Calculations of Sodium Dimer Ion-Pair States
AYDIN SANLI, BEDIHA BESER, JOHN EDWARDSON, Temple University, SYLVIE MAGNIER, Universite Lille, ERGIN AHMED, MARJATTA LYYRA, Temple University — Alkali dimer M2 and alkali hydride MH molecular electronic states with ion-pair character are known to exhibit multiple minima and shoulders in their potential energy curves. This exotic behavior of the of the $1\Sigma^+$ symmetry states is caused by an avoided crossing of the zero-order covalent and ionic (M$^+ + M^-$) potential energy curves. We present a computational study of lifetimes and transition dipole moment matrix elements for the sodium dimer ion-pair states of $1\Sigma^+$ symmetry. We report here the ab initio calculated electric transition dipole moments between the $n \ 1\Sigma^+$ and the $A1\Sigma^+$ states, that vary strongly as a function of internuclear distance. In addition, we have calculated the radiative lifetimes, $\tau$, of these ion-pair states of and compared them with the experimental results from literature when available.

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