BONDING OF ALKALI-ALKALINE EARTH MOLECULES IN THE LOWEST Σ^+ STATES OF DOUBLET AND QUARTET MULTIPLICITY

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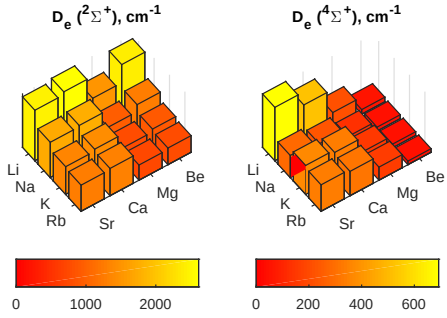
In the present study the ground state as well as the lowest $^4\Sigma^+$ state were determined for 16 AK-AKE molecules.[a] Multireference configuration interaction calculations were carried out in order to understand the bonding of diatomic alkali-alkaline earth (AK-AKE) molecules. The correlations between molecular properties (disociation energy, bond distances, electric dipole moment) and atomic properties (electronegativity, polarizability) will be discussed. A correlation between the dissociation energy and the dipole moment of the lowest $^4\Sigma^+$ state was observed, while the dipole moment of the lowest $^2\Sigma^+$ state does not show such a simple dependency. In this case an empirical relation could be established. The class of AK-AKE molecules was selected for this investigation due to their possible applications in ultracold molecular physics.



[a] J. V. Pototschnig, A. W. Hauser and W. E. Ernst, Phys. Chem. Chem. Phys., 2016,18, 5964-5973