

VIBRONIC TRANSITIONS IN THE X -Sr SERIES (X =Li, Na, K, Rb): ON THE ACCURACY OF NUCLEAR WAVEFUNCTIONS DERIVED FROM QUANTUM CHEMISTRY

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Research on ultracold molecules has seen a growing interest recently in the context of high-resolution spectroscopy and quantum computation. The preparation of molecules in low vibrational levels of the ground state is experimentally challenging, and typically achieved by population transfer using excited electronic states.

On the theoretical side, highly accurate potential energy surfaces are needed for a correct description of processes such as the coherent de-excitation from the highest and therefore weakly bound vibrational levels in the electronic ground state via couplings to electronically excited states. Particularly problematic is the correct description of potential features at large intermolecular distances. Franck-Condon overlap integrals for nuclear wavefunctions in barely bound vibrational states are extremely sensitive to inaccuracies of the potential at long range. In this study, we compare the predictions of common, wavefunction-based ab initio techniques for a known de-excitation mechanism in alkali-alkaline earth dimers. It is the aim to analyze the predictive power of these methods for a preliminary evaluation of potential cooling mechanisms in heteronuclear open shell systems which offer the experimentalist an electric as well as a magnetic handle for manipulation.

The series of X -Sr molecules, with X = Li, Na, K and Rb, has been chosen for a direct comparison. Quantum degenerate mixtures of Rb and Sr have already been produced,^a making this combination very promising for the production of ultracold molecules.

^aB. Pasquiou, A. Bayerle, S. M. Tzanova, S. Stellmer, J. Szczepkowski, M. Parigger, R. Grimm, and F. Schreck, Phys. Rev. A, 2013, 88, 023601