# Excited Electronic States of $Sr_2$: *Ab Initio* Predictions and Experimental Observation of the $2^1\Sigma_u^+$ State

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Despite its apparently simple nature with four valence electrons, the strontium dimer constitutes a challenge for modern electronic structure theory. Here we focus on excited electronic states of $Sr_2$, which we investigate theoretically up to 25000 $cm^{-1}$ above the ground state, to guide and explain new spectroscopic measurements. In particular, we focus on potential energy curves for the $1^1\Sigma_u^+$, $2^1\Sigma_u^+$, $1^1\Pi_u$, $2^1\Pi_u$, and $1^1\Delta_u$ states computed using several variants of *ab initio* coupled-cluster and configuration-interaction methods to benchmark them. In addition, a new experimental study of the excited $2^1\Sigma_u^+$ state using polarisation labelling spectroscopy is presented, which extends knowledge of this state to high vibrational levels, where perturbation by higher electronic states is observed. The available experimental observations are compared with the theoretical predictions and help to assess the accuracy and limitations of employed theoretical models.

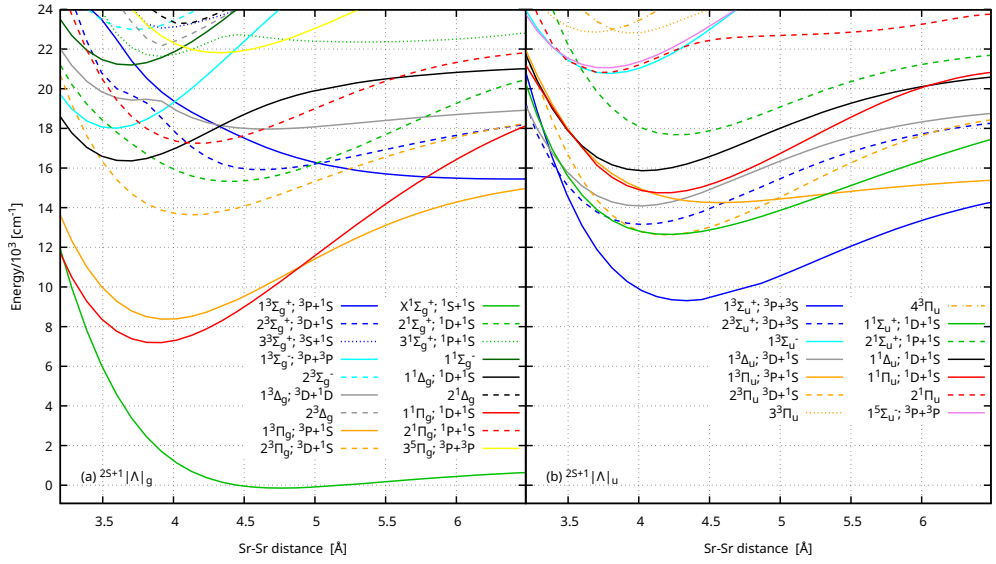


Figure 1: Potential energy curves for the ground and excited electronic states of $Sr_2$ obtained using the non-relativistic spin-free sMRCI+Q/5Z method with the scalar-relativistic small-core pseudopotential.

Financial support from the National Science Centre Poland is gratefully acknowledged: grant no. 2021/43/B/ST4/03326.

[1] J. Szczepkowski, M. Gronowski, A. Grochola, W. Jastrzebski, M. Tomza and P. Kowalczyk, *J. Phys. Chem. A* (2023) available online at doi:10.1021/acs.jpca.3c02056.