

# Unconventional chemistry with alkaline-earth monoxide molecules

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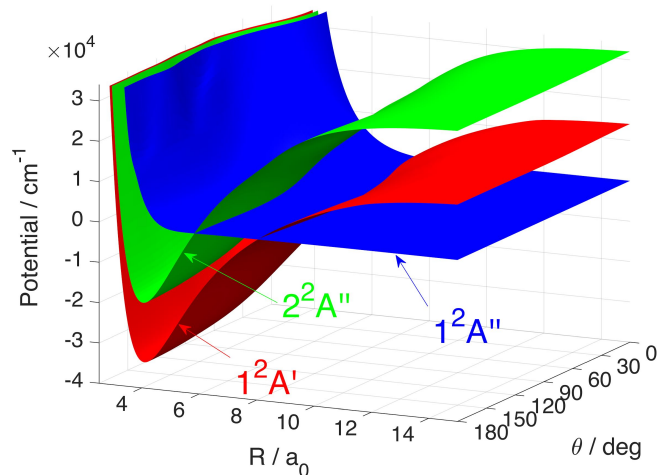
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The interactions of alkaline-earth atoms with inorganic molecules is a fascinating subject with a variety of applications [1]. Of particular interest are alkaline-earth monoxide molecules with a chemical bond that is dominated by a single-valence electron. These molecules are both polar and paramagnetic and thus can be manipulated by electric and magnetic fields as well as laser cooled. An optically-trapped array of such molecules is a candidate for error-free quantum computation. Laser cooling of one such molecule, SrOH, was recently achieved [2].

Here, we report on a quantum mechanical study of the electronic structure of the SrOH molecule using the coupled cluster and the multi-reference configuration-interaction (MRCI) methods of the chemistry package MOLPRO [3]. Complete and accurate information on the SrOH potential surfaces was previously unavailable. We obtained the five energetically-lowest potentials, three are shown in the figure. In the linear geometry with O in the center ( $\theta = 180^\circ$ ) these three potentials have conical intersections, which can facilitate non-adiabatic transitions between electronic states and affect the chemical properties of the molecule. We have located these conical intersections and determined their non-adiabatic couplings.

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FIG. 1. The three energetically-lowest diabatic potentials of SrOH in the  $(R, \theta)$  plane, where  $R$  is the separation between Sr and the center-of-mass of OH and  $\theta$  is the angle between Sr and OH. The OH separation is its equilibrium separation.



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