AN *AB INITIO* STUDY OF ELECTRONICALLY EXCITED STATES OF SiN AND SO

GAP-SUE KIM, *Dharma College, Dongguk University, Seoul, Korea*; RYAN BRADY, NICHOLAS CLARK, WILFRID SOMOGYI, MIKHAIL SEMENOV, SERGEI N. YURCHENKO, *Department of Physics and Astronomy, University College London, London, UK*.

CASSCF + MRCI calculations for the diatomic molecules, SiN and SO, have been performed using the C_{2v} point group symmetry. For SiN, five lowest bound electronic have been were considered, $X\ ^2\Sigma^+$, $A\ ^2\Pi$, $B\ ^2\Sigma^+$, $a\ ^4\Pi$, $b\ ^4\Sigma^+$, while for SO, 9 electronic states were selected, $X\ ^3\Sigma^-$, $A\ ^3\Pi$, $A'\ ^3\Delta$, $A''\ ^3\Sigma^+$, $B\ ^3\Sigma^-$, $C\ ^3\Pi$, $a\ ^1\Delta$, $b\ ^1\Sigma^+$ and $c\ ^1\Sigma^-$, due to their importance for the spectroscopic applications in the IR, Visible and UV regions. For all the excited states potential energy, electronic angular momenta, spin orbit and (transition) dipole moment curves were generated. We use these *ab initio* curves to predict rovibronic spectra of SO and SiN as well as their lifetimes. We aim to construct accurate molecular line lists for these molecules, which will require an empirical refinement of the *ab initio* curves in order to improve the quality of the predictions of experimental spectra.