Aluminium Oxide and Magnesium Oxide, an *ab initio* study

A. T. Patrascu, S. N. Yurchenko, J. Tennyson

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

We present our latest results related to two diatomic oxides: the 21 electron system alluminium oxide (AlO) and the 20 electron system magnesium oxide (MgO). We are interested in these molecules as constituents of the atmospheres of cool stars and (hot) extrasolar planets.
The AlO diatomic molecule is analyzed using several ab initio techniques. The results encompass the lowest 3 electronic states. These are initially generated via a Molpro calculation that produced the uncoupled states along with the associated coupling coefficients (Spin-Orbit, Angular Momentum, Squared Angular Momentum). In order to obtain these states a multi-reference configuration interaction (MRCI) method was used. The total coupled rovibronic states problem is solved variationally. Fitting the *ab initio* potential energy and coupling curves using the available experimental energy levels yields an accurate and stable description of these energy levels and a reliable extrapolation of higher energy levels, not covered by observations. The main tool used for this theoretical description is Duo, an in-house general integrated energy level and line list calculator for diatomic molecules. From the *ab initio* point of view, several numerical methods have been tested including different basis sets (3 to 5 zeta), relativistic corrections (Darwin terms, Douglass Kroll effective Hamiltonians), inclusion of core electron correlations and variations of the active space for the given problem.
For MgO we consider the lowest 4 electronic states. We have started this study with triple and quadrupole-zeta basis sets at the MRCI level and obtain a first estimation of the potential energy curves. We present the potential energy curves obtained systematically using Molpro up to an interatomic distance of 2.5 angstrom. The coupling curves (spin-orbit, angular momentum, squared angular momentum) have been obtained in a similar way. The potential energy curves show peculiar structure at lower energy which makes this molecule an interesting candidate for testing the capabilities of various *ab initio* methods. The latest results will be presented at the conference.

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