

Abstract Submitted  
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***Ab initio* potential curves for the ground states of  $\text{Ca}_2^+$ : Existence of a double minimum in the  $\text{A}^2\Sigma_g^+$  state** SANDIPAN BANERJEE, JASON BYRD, ROBIN CÔTÉ, H MICHELS, JOHN MONTGOMERY, Dept. of Physics, University of Connecticut — We report *ab initio* calculations of the  $\text{X}^2\Sigma_u^+$  and  $\text{A}^2\Sigma_g^+$  states of the  $\text{Ca}_2^+$  dimer. Valence multireference configuration interaction (MRCI) calculations were performed using complete active space self consistent field (CASSCF) orbitals. The CASSCF calculations included all configurations with 3 electrons in 18 valence orbitals and used the aug-cc-pV5Z basis. Core-valence and scalar relativistic effects are included at the CCSDT/cc-pWCVTZ-DK level of theory. A double well, similar to that obtained in recent calculations<sup>1</sup> on  $\text{Be}_2^+$  is found in the  $\text{A}^2\Sigma_g^+$  state. Spectroscopic constants and bound vibrational levels for both the ground states are calculated, as well as Frank-Condon factors and electronic dipole transition moment between the  $\text{X}^2\Sigma_u^+$  and  $\text{A}^2\Sigma_g^+$  states. The static dipole and quadrupole polarizabilities, along with  $C_6$  dispersion coefficient are also reported.

<sup>1</sup>S. Banerjee *et al.* Chem. Phys. Lett. 496 (2010) 208.

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