Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

Potential energy surfaces of metastable CO_2^- for dissociative electron attachment[1] DANIEL HAXTON, Chemical Sciences, Lawrence Berkeley National Lab, C.W. MCCURDY, LBNL; UC Davis, Dept. of Chemistry, TOM RESCIGNO, Lawrence Berkeley National Laboratory, SPIRIDOULA MATSIKA, Temple University — I present potential energy surfaces of the metastable electronic states of the CO_2^- anion relevant to dissociative electron attachment, which proceeds via two electronic states at approximately 4 and 8eV. DEA of CO_2 has been studied by many authors [including Dressler and Allan, Chem Phys 92, 449 (1985); Huels, Parenteau, Cloutier, and Sanche, J Chem Phys 103, 6775 (1995)], but the specific mechanisms of DEA to CO_2 have not been fully elucidated. The anion system is relevant in other contexts including catalytic conversion of CO. In a combined theoretical and experimental study of this system, we have established [J Phys B 44, 205203 (2011)] that the 8eV resonance is indeed a Feshbach resonance of $^2\Pi_g$ symmetry. The system of potential energy surfaces of this pair of states and the pair of states correlating to the 4eV $^2\Pi_u$ shape resonance that is responsible both for DEA and vibrational excitation at this energy, as well as that of the lowest energy anion state that begins as a virtual state at linear geometry and becomes the bound bent CO_2^-, explain the mechanisms of DEA and provide guidance to understand the current results of D. Slaughter, A. Belkacem et al which include angular and kinetic energy distributions of the fragments.

[1]This work was performed under the auspices of the US DOE by LBNL under contract DE-AC02-05CH11231

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Date submitted: 02 Apr 2012 Electronic form version 1.4