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Ab Initio Study of the Use of Ag2- for Catalytic Oxidation of CO. PRATIK DHOLABHAI, XUEYUAN WU, ASOK RAY, Physics Department, The University of Texas at Arlington, 76019 — The formalisms of density functional theory with Perdew and Wang exchange-correlation functional have been employed to study the electronic and geometric structures of silver anion dimer bonded with carbon monoxide and oxygen. Different possible structures for $Ag_2O_2^-$ and Ag_2CO^- have been investigated in detail. An all electron 6-311++G** basis set for carbon and oxygen and a pseudopotential basis set for silver have been used for performing the calculations using the Gaussian 03 suite of programs.[1] Using Ag_2^- as a catalyst, a full catalytic cycle producing two CO_2 molecules will be presented. Also, presence of an intermediate state, $Ag_2CO_3^-$, which can be detected experimentally, is predicted. Presence of an energy barrier for certain reactions from the catalytic cycle has *not* been observed. This is noteworthy since it has been claimed in the literature that for the same catalytic cycle to proceed using Au_2^- as a catalyst, it has to overcome an energy barrier. Charge state effects have been studied by following similar steps for the catalytic cycle using the Ag_2^+ and Ag_2 as catalysts. We conclude that the Ag_2^- performs better as a catalyst compared to the Ag_2^+ and Ag_2. *****Work supported, in part, by the Welch Foundation, Houston, Texas (Grant No. Y-1525). [1] *Gaussian 03,* M. J. Frisch *et al.,* Gaussian Inc., Pittsburgh, PA.

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