Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

High pressure studies on extended phases of CO_2 JAVIER A. MONTOYA, Princeton University, MAL-SOON LEE, Michigan State University, SANDRO SCANDOLO, Abdus Salam International Centre for Theoretical Physics — Recent findings have shown that the chemistry of CO_2 at high pressure and temperature is richer than previously thought and that the activation of the C=O bond that can give origin to different forms of non-molecular CO_2. Such findings may have important implications for the understanding of the Earth's deep carbon cycle and CO_2 sequestration technologies. First principles simulations of CO_2's electronic properties under different pressure and temperature conditions can constrain the thermodynamic phase diagram of CO_2 and explore P-T conditions necessary for the C=O bond activation. We have shown that at about 50 GPa molecular CO_2 can transform to a metastable amorphous form characterized by an almost equal proportion of three- and four-fold coordinated carbon atoms [1], while higher carbon coordination does not take place up to at least 900 GPa [2-3]. We have also found that doping with transition metals can reduce the activation barrier and transition pressure for the C=O bond activation in CO_2 [4]. Our results suggest that pressure can radically alter the oxidation chemistry of carbon. [1] J. A. Montoya *et al.*, PRL 100, 163002 (2008) [2] J. Sun et al., PNAS 106, 6077 (2009) [3] M-S. Lee, J. A. Montoya and S. Scandolo, PRB 79, 144102 (2009) [4] J. A. Montoya, R. Rousseau, and S. Scandolo, unpublished.

Javier A. Montoya
Princeton University

Date submitted: 20 Nov 2009 Electronic form version 1.4