Abstract Submitted
for the DAMOP16 Meeting of
The American Physical Society

Theoretical and Experimental Evidence of Hydrogen Migration rather than Isomerization in the Acetylene Dication[1] CHELSEA LIEKHUS-SCHMALTZ, ZHENG LI, VLADIMIR PETROVIC, TODD MARTINEZ, PHIL BUCKSBAUM, Stanford University, Pulse Institute, AMO75113 COLLABORATION — Theoretical calculations and experimental results in the acetylene dication have long agreed that isomerization after x-ray excitation occurs in the first singlet state, where the carbon-carbon bond lives long enough for isomerization to complete [1]. These same calculations predict that a large barrier to isomerization exists that would cause isomerization to occur in about a picosecond, while there is some evidence for ultrafast isomerization in under 100 fs. However, new ab initio calculations of the acetylene dication reveal that ultrafast isomerization after x-ray excitation is unlikely. In this talk, we present evidence that signatures of hydrogen migration observed in recent time resolved LCLS data [2] are mostly due to hydrogen migration in an excited state which dissociates too quickly for isomerization to complete. [1] T. S. Zyubina, Y. A. Dyakov, S. H. Lin, A. D. Bandrauk, and A. M. Mebel., "Theoretical study of isomerization and dissociation of acetylene dication in the ground and excited electronic states," J. Chem. Phys. **123**, 134320 (2005). [2] C. E. Liekhus-Schmaltz, et al, "Ultrafast isomerization initiated by X-ray core ionization," Nat. Commun. **6**, 8199 (2015).

[1] This material is based upon work supported by the National Science Foundation under Grant No. PHY-0649578.

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Date submitted: 28 Jan 2016 Electronic form version 1.4