Supplementary Information (SI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2024

Supporting Information

Time-resolved photoelectron-diffraction imaging of methanol photodissociation involving molecular-hydrogen ejection

Kazuki Yoshikawa,[†] Manabu Kanno,[*,‡] Hao Xue,[‡] Naoki Kishimoto,[*,‡] Soki Goto,[¶] Fukiko Ota,[¶] Yoshiaki Tamura,[¶] Florian Trinter,[*,§,‖] Kilian Fehre,[‖] Leon Kaiser,[‖] Jonathan Stindl,[‖] Dimitrios Tsitsonis,[‖] Markus Schöffler,[‖] Reinhard Dörner,[‖] Rebecca Boll,[⊥] Benjamin Erk,[#] Tommaso Mazza,[⊥] Terence Mullins,[⊥] Daniel E. Rivas,[⊥] Philipp Schmidt,[⊥] Sergey Usenko,[⊥] Michael Meyer,[⊥] Enliang Wang,[@] Daniel Rolles,[@] Artem Rudenko,[@] Edwin Kukk,[△] Till Jahnke,[⊥,∇] Sergio Díaz-Tendero,[*,††,‡‡,¶¶] Fernando Martín,[††,§§] Keisuke Hatada,[*,¶] and Kiyoshi Ueda[*,‡,‖‖]

†*Department of Physics, University of Toyama, Gofuku 3190, Toyama 930-8555, Japan*

‡*Department of Chemistry, Tohoku University, 6-3 Aramaki Aza-Aoba, Aoba-ku, Sendai 980-8578, Japan*

¶*Department of Physics, University of Toyama, Gofuku 3190, Toyama 930-8555, Japan*

§*Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*

‖*Institut für Kernphysik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany*

⊥*European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany*

#*FLASH, DESY, Notkestraße 85, 22607 Hamburg, Germany*

@*J.R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA*

△*Department of Physics and Astronomy, University of Turku, FI-20014 Turku, Finland*

∇*Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*

††*Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain*

‡‡*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain*

¶¶*Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain*

§§*Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nano), Campus de Cantoblanco, 28049 Madrid, EU, Spain*

‖‖*School Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China*

E-mail: manabu.kanno.d2@tohoku.ac.jp; kishimoto@tohoku.ac.jp; trinter@fhi-berlin.mpg.de; sergio.diaztendero@uam.es; hatada@sci.u-toyama.ac.jp; kiyoshi.ueda@tohoku.ac.jp

Figures S.1, S.2, and S.3 show PA-MFPADs for an arbitrary single trajectory of the fragmentation channels $CHO^+ + H_2 + A^+$, as example 1, example 2, and example 3, respectively, at photoelectron energies of (a) 100 eV, (b) 500 eV, and (c) 2.5 keV after the formation of the doubly charged methanol ion. The color codes for the atoms in the figures are oxygen - green, carbon - white, and hydrogen – blue. To guide the eye, two arrows (in each time frame) indicate the position of the peaks associated with two hydrogen atoms, which ultimately become H_2. We set the O atom at the origin, the C atom on the z axis ($z > 0$), and the center of mass of the ejected H_2 on the zx plane ($x > 0$). We see how the two H atoms come together.

Figure S.4 shows the temporal evolution of the PA-MFPADs averaged over 200 trajectories for H_2 ejection at photoelectron energies of (a) 100 eV, (b) 500 eV, and (c) 2.5 keV after the formation of the doubly charged methanol ion. The same reaction plane is used as in the previous figures. In this figure, the PA-MFPADs are viewed from the positive z axis to see the two H atoms approach $y = 0$ over time. The arrows (in each time frame) indicate the angles averaged over 200 trajectories for the position of H atoms, which ultimately become H_2.

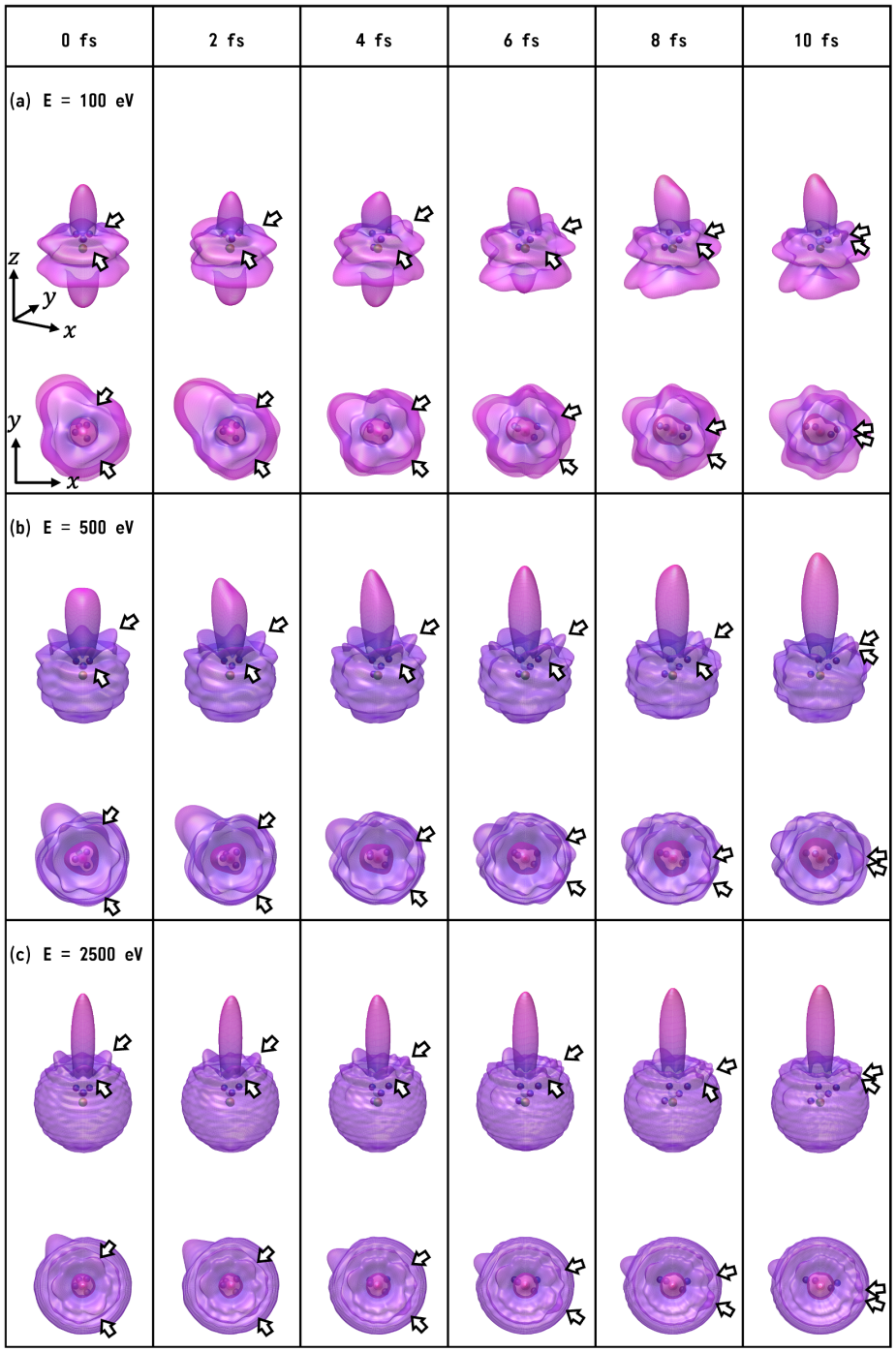

Figure S.1: Snapshots of a single-trajectory PA-MFPAD (example 1) for H_2 ejection at photoelectron energies (a) 100 eV, (b) 500 eV, and (c) 2.5 keV. Color code for the atoms: oxygen - green, carbon - white, and hydrogen – blue. To guide the eye, two arrows (in each time frame) indicate the position of the peaks associated with two hydrogen atoms, which ultimately become H_2. We set the O atom at the origin, the C atom on the z axis ($z > 0$), and the center of mass of the ejected H_2 on the zx plane ($x > 0$).

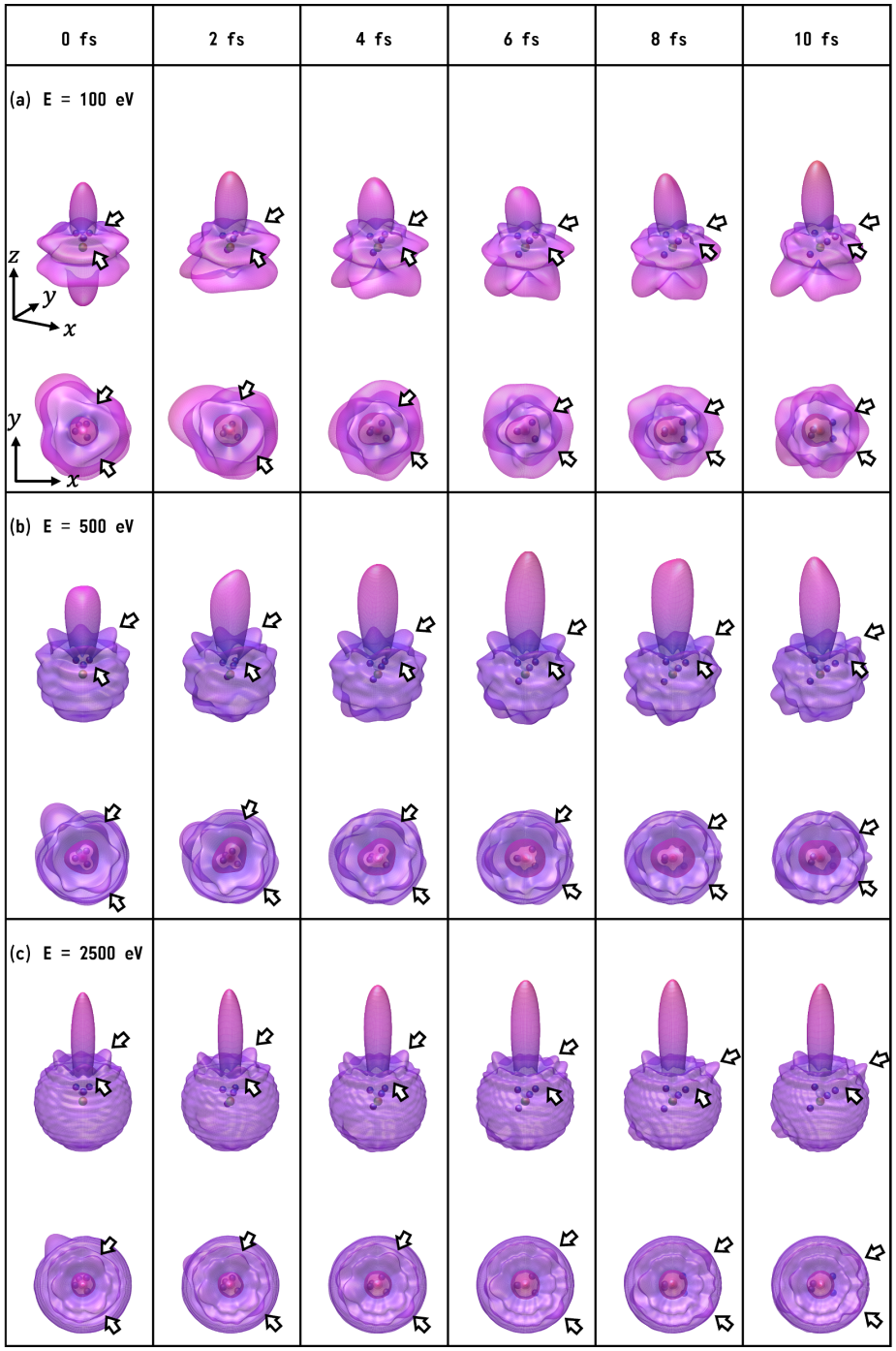

Figure S.2: Snapshots of a single-trajectory PA-MFPAD (example 2) for H_2 ejection at photoelectron energies (a) 100 eV, (b) 500 eV, and (c) 2.5 keV. Color code for the atoms: oxygen - green, carbon - white, and hydrogen – blue. To guide the eye, two arrows (in each time frame) indicate the position of the peaks associated with two hydrogen atoms, which ultimately become H_2. We set the O atom at the origin, the C atom on the z axis ($z > 0$), and the center of mass of the ejected H_2 on the zx plane ($x > 0$).

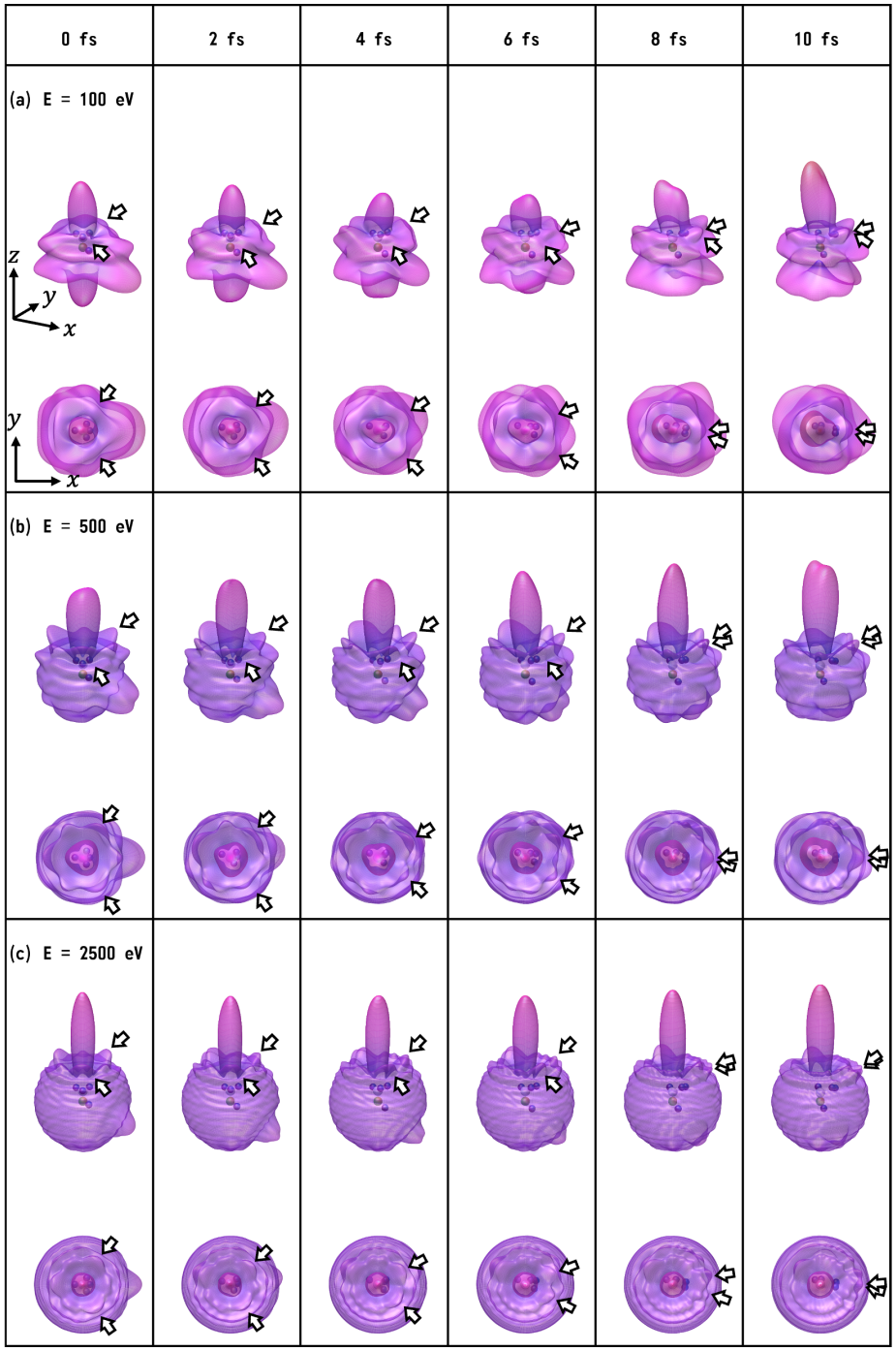

Figure S.3: Snapshots of a single-trajectory PA-MFPAD (example 3) for H_2 ejection at photoelectron energies (a) 100 eV, (b) 500 eV, and (c) 2.5 keV. Color code for the atoms: oxygen - green, carbon - white, and hydrogen – blue. To guide the eye, two arrows (in each time frame) indicate the position of the peaks associated with two hydrogen atoms, which ultimately become H_2. We set the O atom at the origin, the C atom on the z axis ($z > 0$), and the center of mass of the ejected H_2 on the zx plane ($x > 0$).

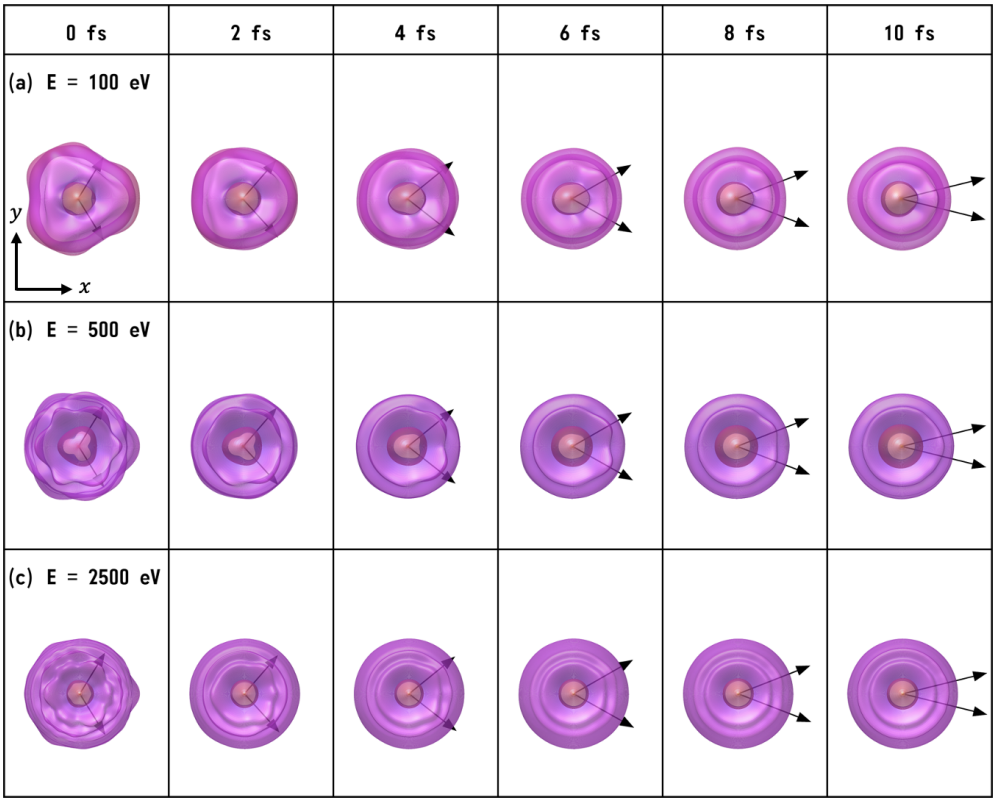

Figure S.4: Snapshots of PA-MFPADs averaged over 200 trajectories for H_2 ejection at photoelectron energies (a) 100 eV, (b) 500 eV, and (c) 2.5 keV. The arrows (in each time frame) indicate the angles averaged over 200 trajectories for the position of H atoms which ultimately become H_2. We set the O atom at the origin, the C atom on the z axis ($z > 0$), and the center of mass of the ejected H_2 on the zx plane ($x > 0$).