

## Appendix A

# Experimental Pulse Parameters

Table A.1 summarizes the IR-pulse parameters of the experiments leading to the results presented in Chaps. 3 and 4, i.e., the center frequency  $\nu$ , bandwidth  $\Delta\nu$  (FWHM) and pulse energy  $E$  of the pulses  $k_1$ ,  $k_2$  and  $k_3$  in 2D IR experiments and of pump and probe pulses in pump-probe experiments. We deduced probe-pulse energies on the order of 10 nJ by assuming that  $\approx 2\%$  of the pulse energy are reflected by the BaF<sub>2</sub> wedge. The time resolution  $T_{res}$  was estimated from FROG traces generated in CaF<sub>2</sub> or ZnSe windows (2D IR) or cross-correlation traces, e.g., measured by the instantaneous response of semiconductor materials (pump probe).

The sample thickness  $d$  depends on the vibrational marker mode used and the water content (for measurements of the ultrafast dynamics of OH stretching or bending vibrations). BaF<sub>2</sub> windows were used for experiments of the phosphate stretching vibration due to their lower dispersion compared to CaF<sub>2</sub> in the frequency range of 1000–1250 cm<sup>-1</sup>. The thickness of the BaF<sub>2</sub> and CaF<sub>2</sub> windows was 1 mm. For the two-color experiments of Sect. 4.1.1 we used 500 nm thick Si<sub>3</sub>N<sub>4</sub> windows in order to suppress nonresonant signals from coherent pump-probe coupling in the sample windows.

**Table A.1** Pulse parameters: Central frequency  $\nu$ , bandwidth  $\Delta\nu$  (FWHM), pulse energy  $E$  and time resolution  $T_{res}$  of the experiment. For the sake of completeness, the sample thickness  $d$  and the window material are given as well

Section	Pulse	$\nu$ (cm <sup>-1</sup> )	$\Delta\nu$ (cm <sup>-1</sup> )	$E$ ( $\mu$ J)	$T_{res}$ (fs)	$d$ ( $\mu$ m)	Window
3.1	$k_{1,2,3}$	1090–1260	170–200	0.8	<150	25	BaF <sub>2</sub>
	pump	1100/1260	120/180	1.4/2.4	<300/<200	25	BaF <sub>2</sub>
3.2	probe	1130/1260	180/180	$\approx 10^{-2}$			
	pump	1760	160	0.8	$\approx 200$	25	CaF <sub>2</sub>
3.3	probe	1780	200	$\approx 10^{-2}$			
	pump	3400	340	$\approx 0.5$	<80	100 ( $w_0 = 1$ )	CaF <sub>2</sub>
4.1	pump	3400	180	1.8	<150	25 ( $w_0 = 5, 8$ )	
	probe	3400	350	$\approx 10^{-2}$		6 ( $w_0 = 16$ )	
4.1.1	pump	3410	190	2.0	130	200	Si <sub>3</sub> N <sub>4</sub>
	probe	1690	240	$\approx 10^{-2}$			
4.2	pump	1635	100	2.5	140	200 ( $w_0 = 2, 3$ )	CaF <sub>2</sub>
	probe	1670	240	$\approx 10^{-2}$		100 ( $w_0 = 8$ )	
4.3	pump	3410	200	2	170	50 ( $w_0 = 16$ )	CaF <sub>2</sub>
	probe	3300	350	$\approx 10^{-2}$		25 ( $w_0 = 3$ )	
4.3	pump	3420	270	2.5	$\approx 250$	6 ( $w_0 = 16$ )	BaF <sub>2</sub>
	probe	1270	160	$\approx 10^{-2}$		25 ( $w_0 = 16$ )	

# Curriculum Vitae

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## Education and scientific career:

- 2014– Postdoctoral researcher at the Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie (MBI): Ultrafast vibrational dynamics in biomolecules and solids
- 2010–2014 Graduate student at MBI: Ultrafast hydrogen-bond dynamics and energy dissipation in hydrated biomolecular systems using time-resolved vibrational spectroscopy, in particular two-dimensional infrared methods
- 2009–2010 Staff member at MBI: Implementation of a new laboratory for time-resolved mid-infrared spectroscopy
- 2008–2009 Master student at MBI: Shaping and characterization of ultrashort mid-infrared pulses
- 2004–2009 Studies of physics at Humboldt University (Berlin), degree: Diplom-Physiker

## Publications

### Peer-reviewed articles:

- R. Costard, I. A. Heisler, and T. Elsaesser. “Structural dynamics of hydrated phospholipid surfaces probed by ultrafast 2D spectroscopy of phosphate vibrations”. *J. Phys. Chem. Lett.* 5 (2014), 506–511.
- R. Costard and T. Elsaesser. “Femtosecond OH bending dynamics of water nanopools confined in reverse micelles”. *J. Phys. Chem. B* 117 (2013), 15338–15345.
- R. Costard, C. Greve, I. A. Heisler, and T. Elsaesser. “Ultrafast energy redistribution in local hydration shells of phospholipids: A two-dimensional infrared study”. *J. Phys. Chem. Lett.* 3 (2012), 3646–3651.
- R. Costard, N. E. Levinger, E. T. J. Nibbering, and T. Elsaesser. “Ultrafast vibrational dynamics of water confined in phospholipid reverse micelles”. *J. Phys. Chem. B* 116 (2012), 5752–5759.
- N. E. Levinger, R. Costard, E. T. J. Nibbering, and T. Elsaesser. “Ultrafast energy migration pathways in self-assembled phospholipids interacting with confined water”. *J. Phys. Chem. A* 115 (2011), 11952–11959.
- R. Costard, T. Tyborski, B. P. Fingerhut, and T. Elsaesser. “Ultrafast phosphate hydration dynamics in bulk H<sub>2</sub>O”. *J. Chem. Phys.* (accepted).
- R. Costard, C. Greve, H. Fidder, and E. T. J. Nibbering. “Hydrogen bonding induced enhancement of Fermi resonances: Ultrafast vibrational energy flow dynamics in aniline-d<sub>5</sub>”. *J. Phys. Chem. B* (in press).
- T. Tyborski, R. Costard, M. Woerner, and T. Elsaesser. “Ultrafast vibrational dynamics of BH<sub>4</sub><sup>-</sup> ions in liquid and crystalline environments”. *J. Chem. Phys.* 141 (2014), 034506.
- C. Greve, N. K. Preketes, H. Fidder, R. Costard, B. Koeppe, I. A. Heisler, S. Mukamel, F. Temps, E. T. J. Nibbering, and T. Elsaesser. “N-H stretching excitations in adenosine-thymidine base pairs in solution: Pair geometries, infrared line shapes, and ultrafast vibrational dynamics”. *J. Phys. Chem. A* 117 (2013), 594–606.
- C. Greve, N. K. Preketes, R. Costard, B. Koeppe, H. Fidder, E. T. J. Nibbering, F. Temps, S. Mukamel, and T. Elsaesser. “N-H stretching modes of adenosine monomer in solution studied by ultrafast nonlinear infrared spectroscopy and ab initio calculations”. *J. Phys. Chem. A* 116 (2012), 7636–7644.

### Conference proceedings:

- R. Costard, C. Greve, N. E. Levinger, E. T. J. Nibbering, and T. Elsaesser. “Ultrafast vibrational dynamics of water confined in phospholipid reverse micelles”. *EPJ Web Conf.* 41 (2013), 06003.
- C. Greve, N. K. Preketes, R. Costard, B. Koeppe, H. Fidder, E. T. J. Nibbering, F. Temps, S. Mukamel, and T. Elsaesser. “Ultrafast IR pump-probe and 2D-IR photon echo spectroscopy of adenosine-thymidine base pairs”. *EPJ Web Conf.* 41 (2013), 05019.

- C. Greve, R. Costard, H. Fidder, and E. T. J. Nibbering. “Hydrogen bond enhancement of Fermi resonances explored with ultrafast IR two-colour pump-probe and 2D-IR spectroscopy”. *Ultrafast Phenomena XIX*. ed. by K. Yamanouchi, S. Cundiff, R. Vivie-Riedle, M. Kuwata-Gonokami, and L. DiMauro. Vol. 162. Springer Proc. Phys. 2015, 471–474.
- R. Costard, I. A. Heisler, and T. Elsaesser. “Hydrated phospholipid surfaces probed by ultrafast 2D spectroscopy of phosphate vibrations”. *Ultrafast Phenomena XIX*. ed. by K. Yamanouchi, S. Cundiff, R. Vivie-Riedle, M. Kuwata-Gonokami, and L. DiMauro. Vol. 162. Springer Proc. Phys. 2015, 301–304.

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