Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: An *On-the-Fly* Deep Neural Network for Simulating Time-Resolved Spectroscopy: Predicting the Ultrafast Ring Opening Dynamics of 1,2-Dithiane

Table S1: The percentage error for the whole trajectory and 4 time windows: **I** (100-300 fs), **II** (300-500 fs), **III** (500-700 fs) and **IV** (700-900 fs) for each trajectory not shown in the main text.

Trajectory	Overall	**I**	**II**	**III**	**IV**	Trajectory	Overall	**I**	**II**	**III**	**IV**
4	12.9	7.0	15.3	12.2	17.2	28	18.2	5.1	19.9	22.1	25.5
5	10.0	6.7	12.5	10.9	9.7	29	9.3	1.3	11.9	13.0	11.0
6	9.7	3.2	16.2	7.6	11.6	30	11.1	9.1	8.2	14.0	13.0
7	12.3	8.1	14.7	11.9	14.3	31	14.1	10.3	14.5	18.8	12.7
8	7.8	3	10.5	6.2	11.4	32	18.0	8.3	18.2	23.1	22.2
9	14.7	5.6	15.7	18.6	18.9	33	8.3	6.3	8.0	7.8	11.1
10	9.4	7.4	12.0	8.5	9.5	34	7.8	5.0	9.5	6.3	10.3
11	11.0	4.3	8.7	15.2	15.7	35	11.7	5.0	17.9	12.6	11.4
12	9.9	7.0	6.7	13.6	12.3	36	6.7	2.3	8.8	8.9	6.9
13	9.0	3.9	8.8	10.3	13.2	37	10.4	2.4	11.2	9.3	18.7
14	9.5	6.3	11.3	8.3	12.0	38	9.7	7.4	9.6	9.7	12.1
15	11.5	8.9	16.0	10.3	10.7	39	12.0	6.6	13.5	13.0	14.8
16	14.6	7.2	13.0	18.7	19.3	40	12.0	6.3	13.3	15.7	12.5
17	10.3	4.7	11.6	10.7	14.1	41	10.7	5.9	11.2	11.6	14.1
18	7.1	2.3	7.8	11.2	7.2	42	9.9	3.8	11.3	11.1	13.3
19	11.9	4.8	10.3	16.9	15.4	43	11.2	0.1	17.6	10.3	16.8
20	7.9	5.1	6.3	12.1	8.0	44	9.0	6.2	10.6	8.7	10.6
21	10.7	10.7	10.0	12.8	9.4	45	8.6	1.9	8.8	8.4	12.6
22	8.0	3.4	8.9	10.3	9.5	46	11.5	9.2	13.3	12.6	10.9
23	9.2	4.4	10.3	9.9	12.2	47	8.2	4.4	7.6	11.3	9.5
24	6.9	1.5	6.8	9.9	9.4	48	8.3	3.9	10.7	8.6	10.0
25	8.1	2.4	9.4	8.2	12.4	49	7.9	3.5	6.3	10.2	11.5
26	9.9	4.8	10.4	10.6	13.6	50	9.4	5.5	11.6	8.8	11.7
27	11.1	4.2	13.8	12.1	14.2	51	7.7	3.3	9.3	7.8	10.5

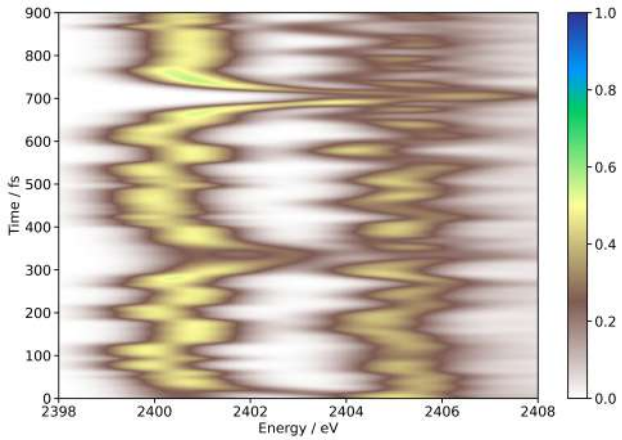

Figure S1: Trajectory 1: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

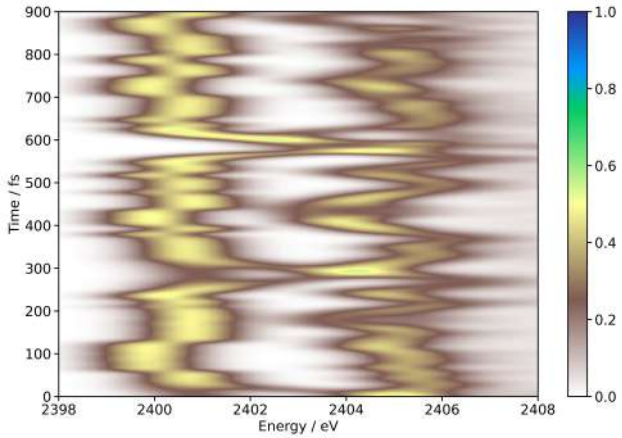

Figure S2: Trajectory 2: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

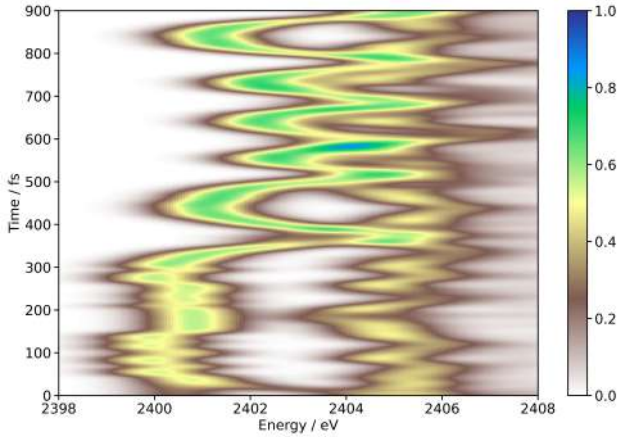

Figure S3: Trajectory 3: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

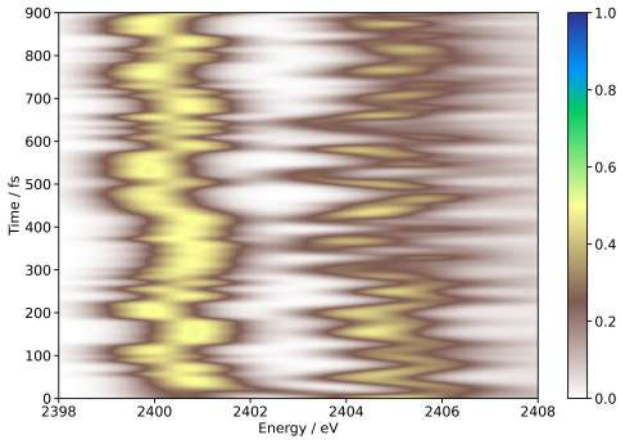

Figure S4: Trajectory 4: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

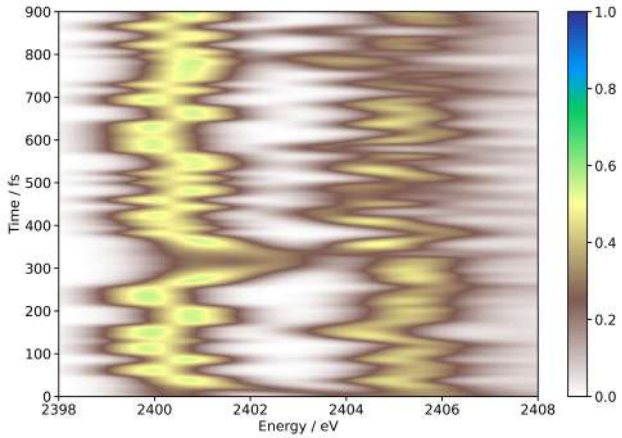

Figure S5: Trajectory 5: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

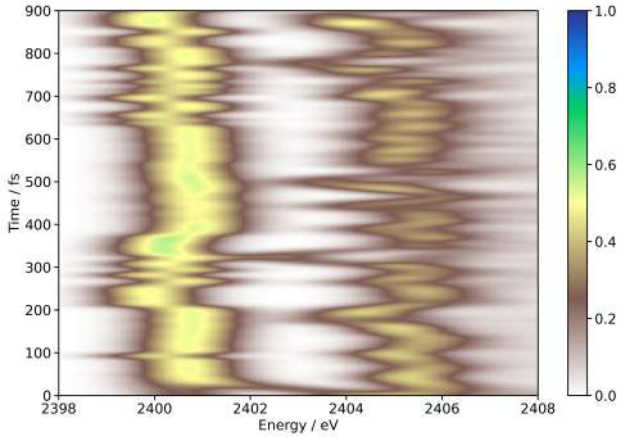

Figure S6: Trajectory 6: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

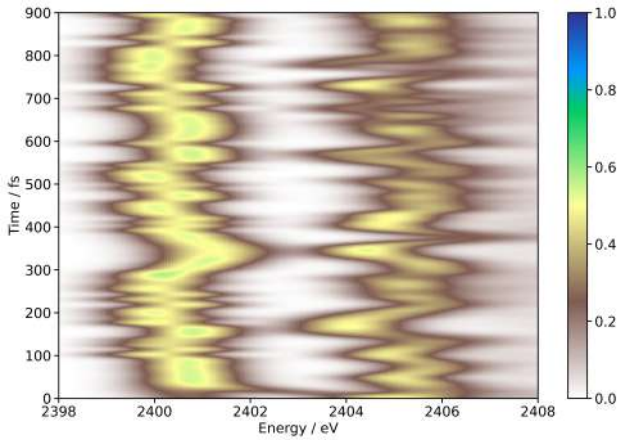

Figure S7: Trajectory 7: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

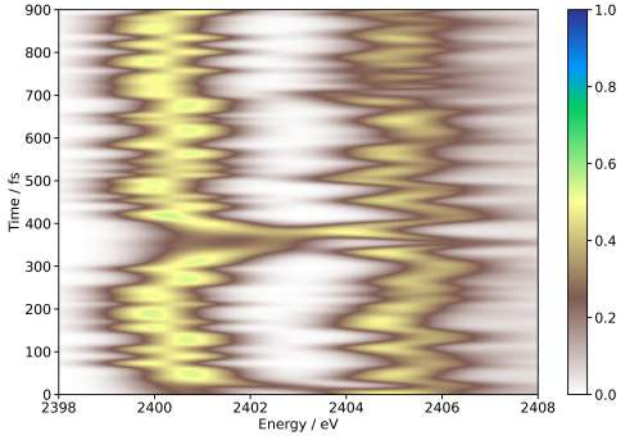

Figure S8: Trajectory 8: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

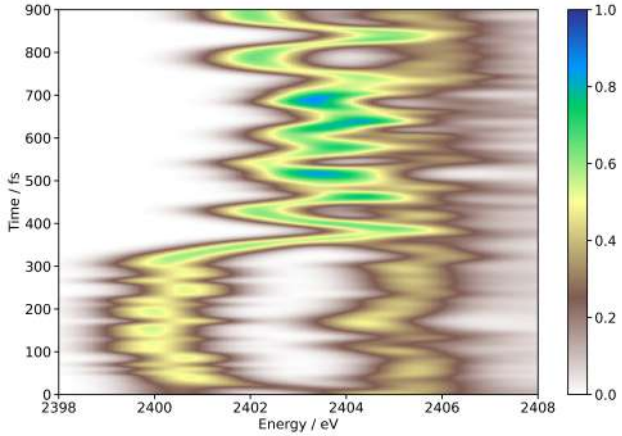

Figure S9: Trajectory 9: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

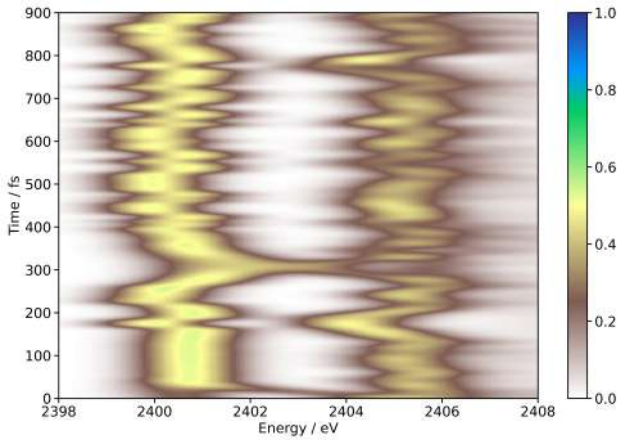

Figure S10: Trajectory 10: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

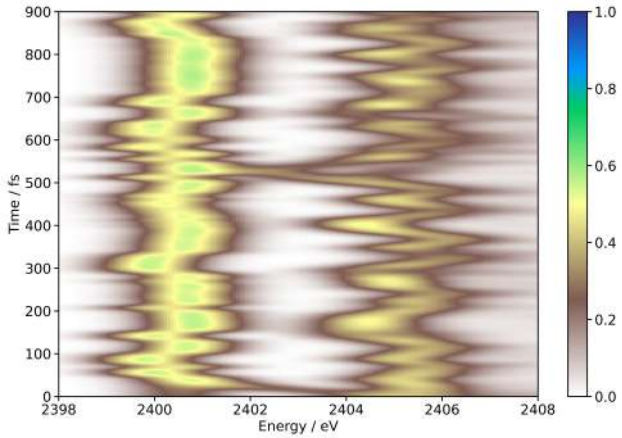

Figure S11: Trajectory 11: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

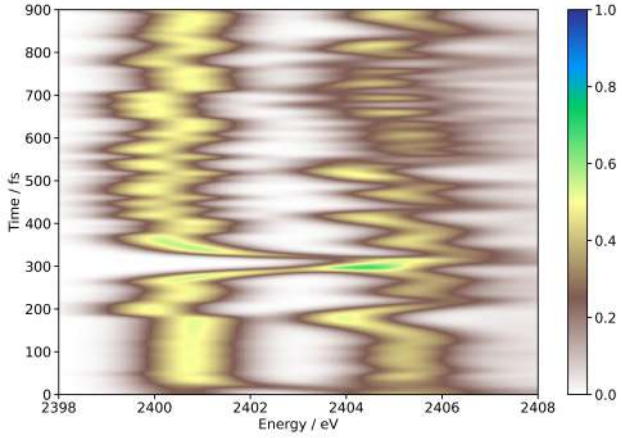

Figure S12: Trajectory 12: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

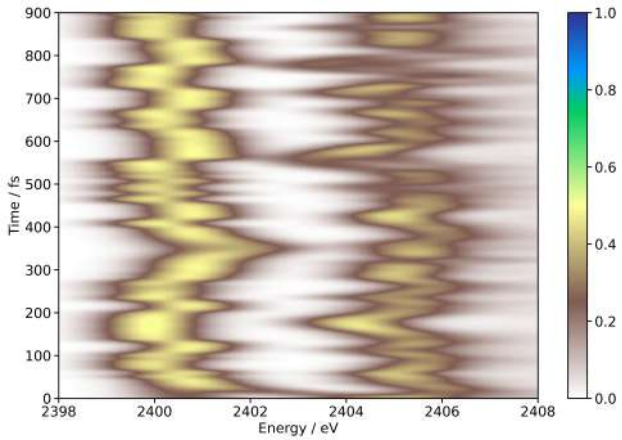

Figure S13: Trajectory 13: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

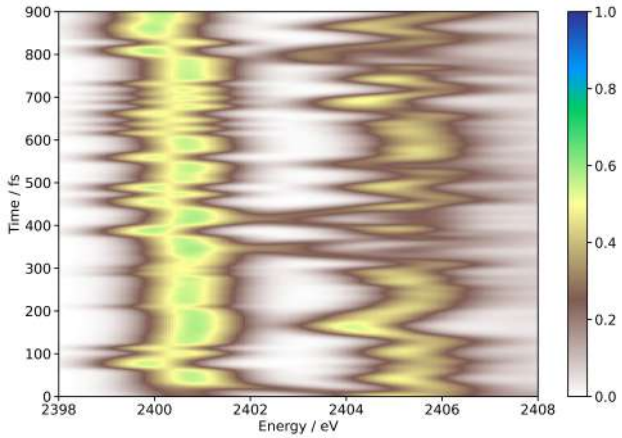

Figure S14: Trajectory 14: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

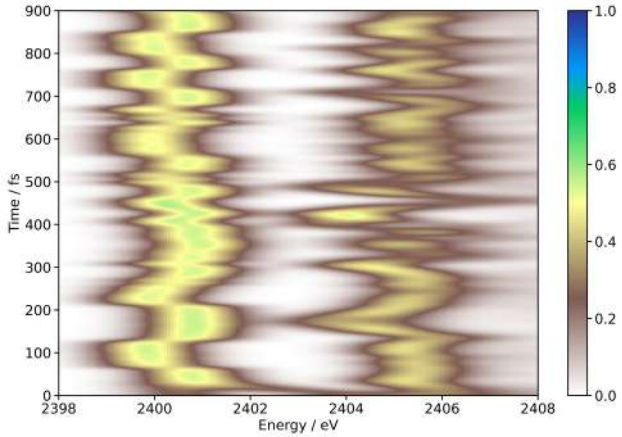

Figure S15: Trajectory 15: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

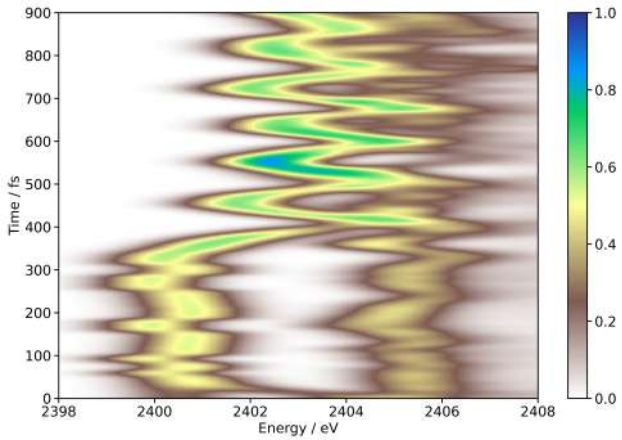

Figure S16: Trajectory 16: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

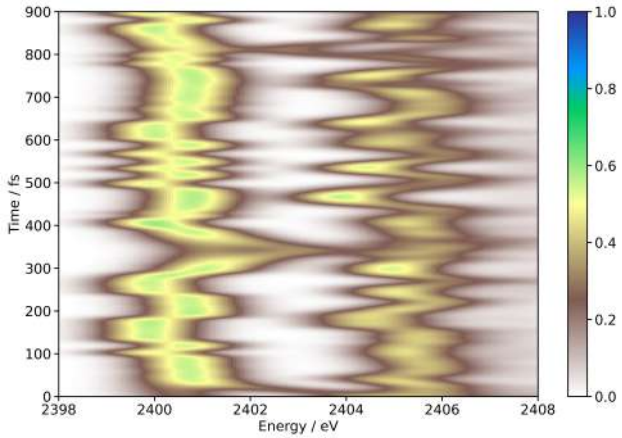

Figure S17: Trajectory 17: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

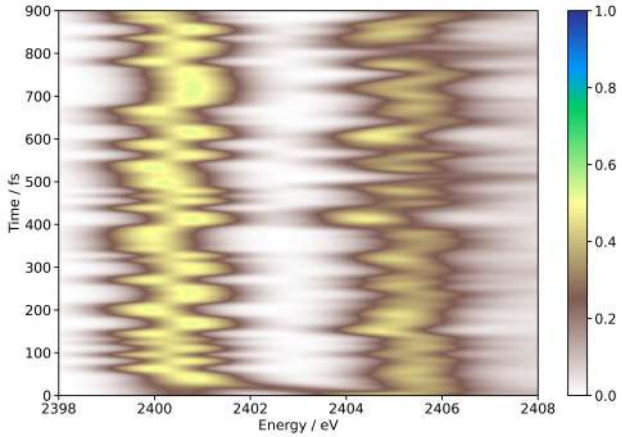

Figure S18: Trajectory 18: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

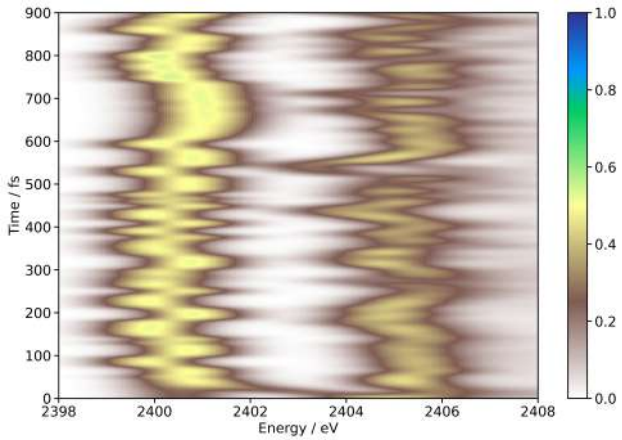

Figure S19: Trajectory19: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

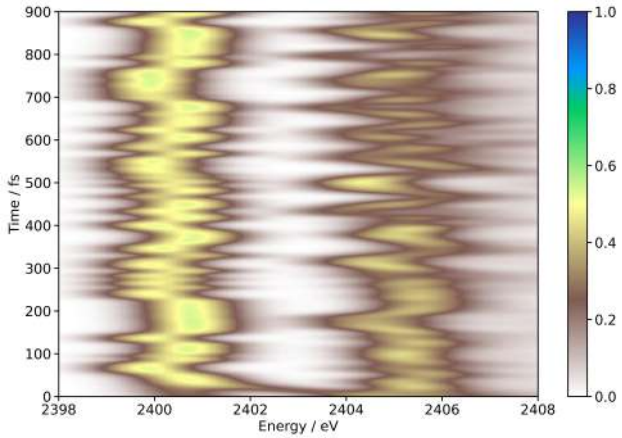

Figure S20: Trajectory 20: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

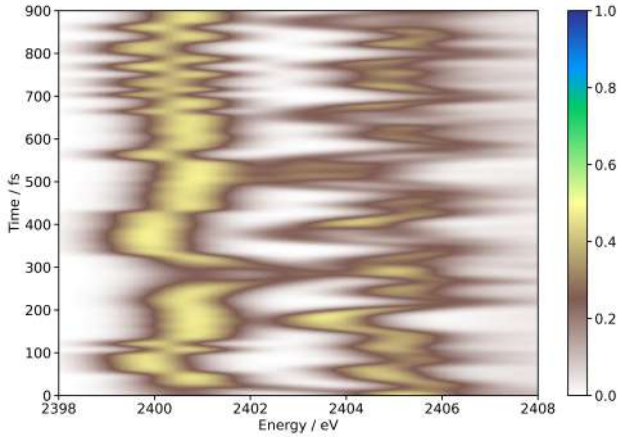

Figure S21: Trajectory 21: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

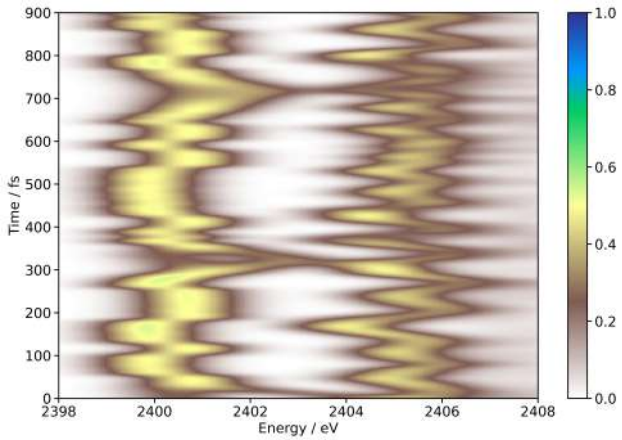

Figure S22: Trajectory 22: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

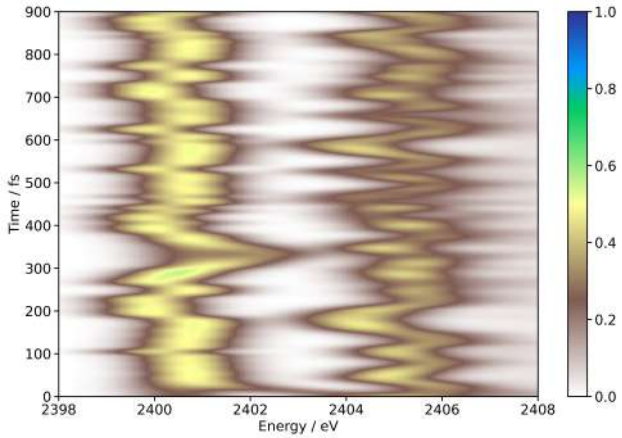

Figure S23: Trajectory 23: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

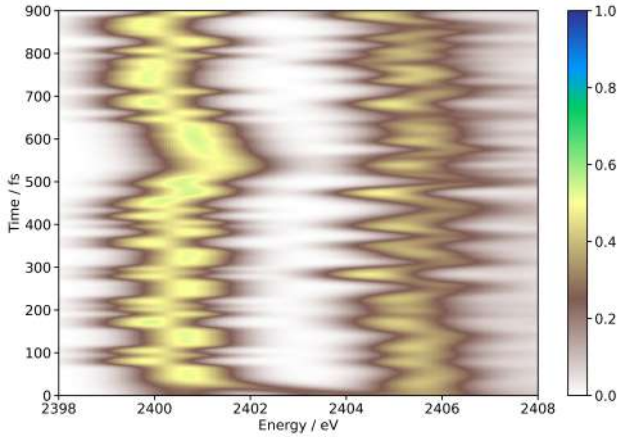

Figure S24: Trajectory 24: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

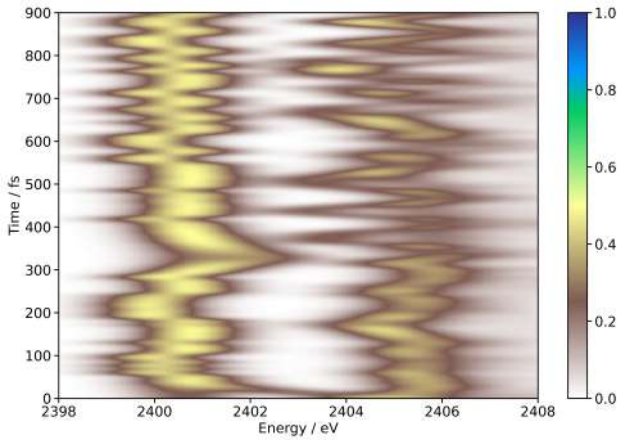

Figure S25: Trajectory 25: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

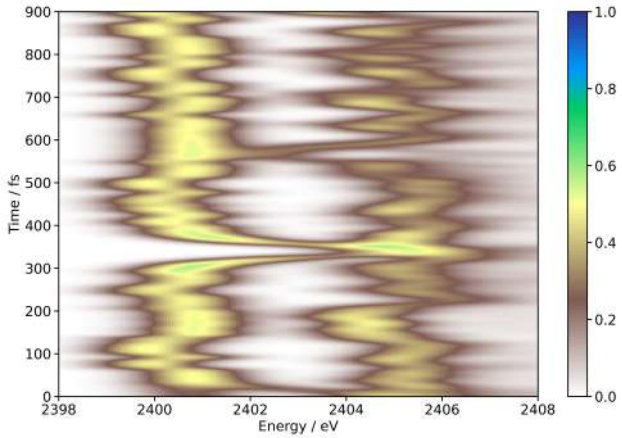

Figure S26: Trajectory 26: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

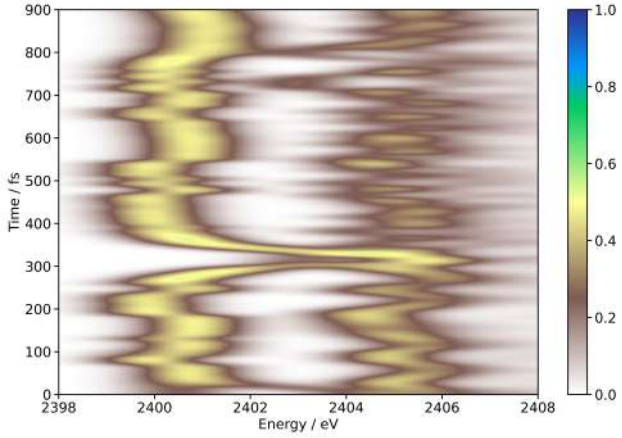

Figure S27: Trajectory 27: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

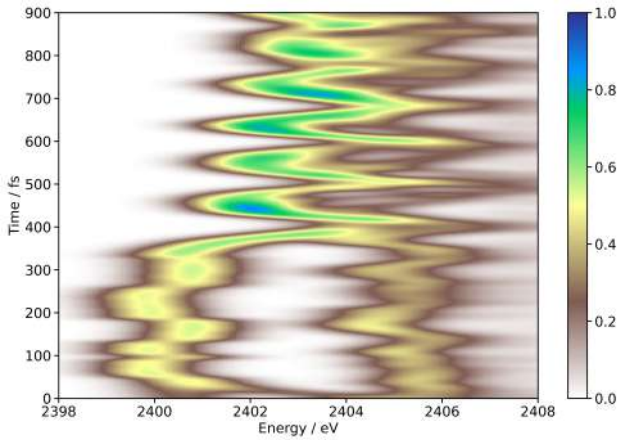

Figure S28: Trajectory 28: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

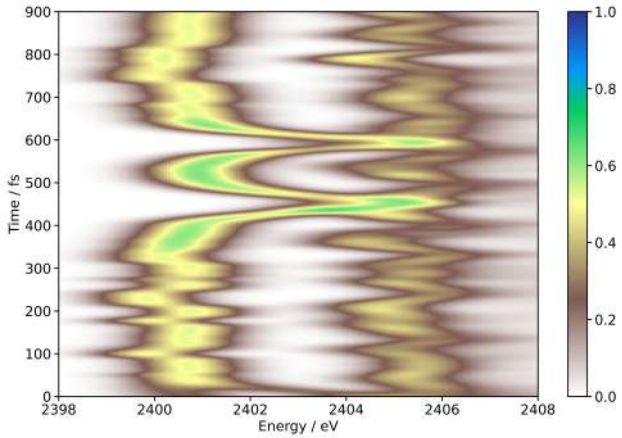

Figure S29: Trajectory 29: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

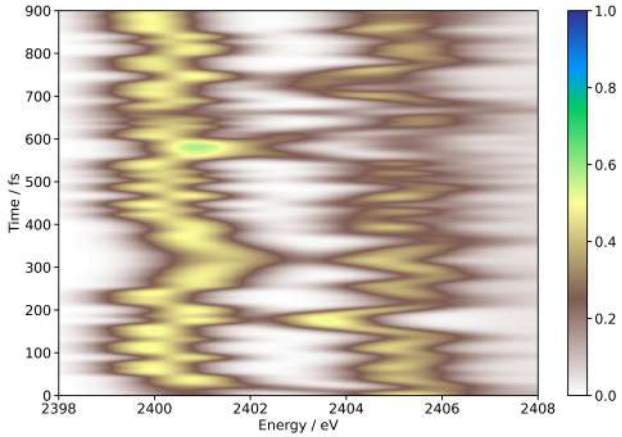

Figure S30: Trajectory 30: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

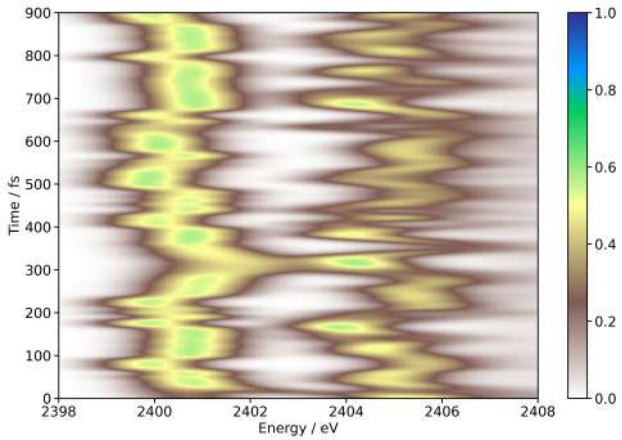

Figure S31: Trajectory 31: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

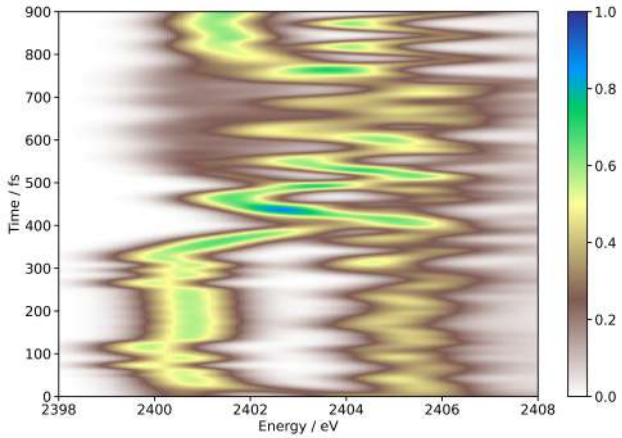

Figure S32: Trajectory 32: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

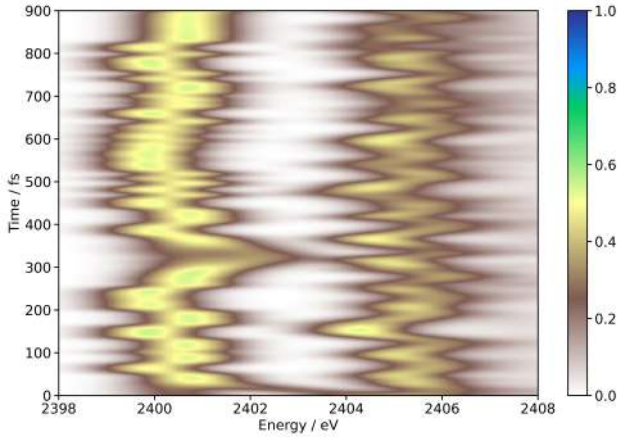

Figure S33: Trajectory 33: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

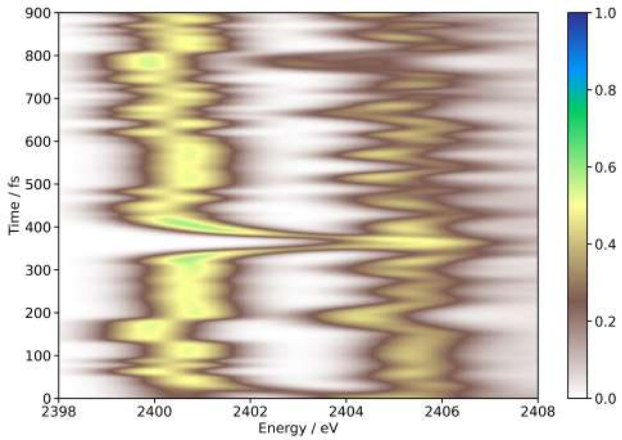

Figure S34: Trajectory 34: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

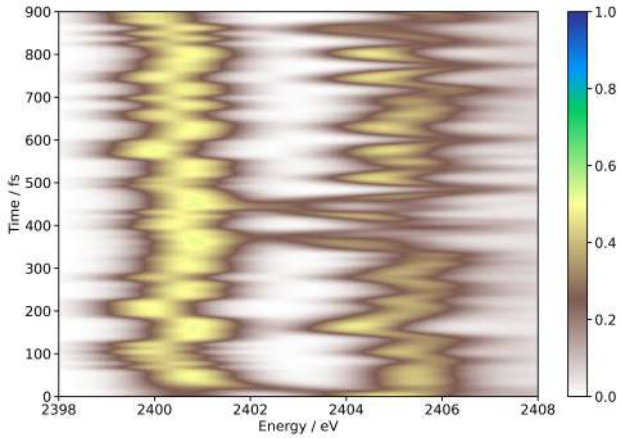

Figure S35: Trajectory 35: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

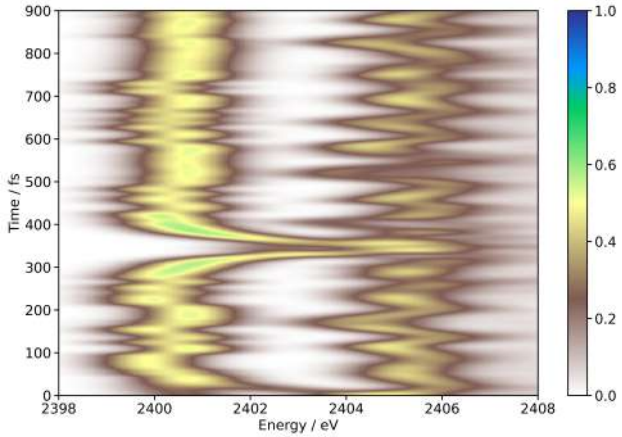

Figure S36: Trajectory 36: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

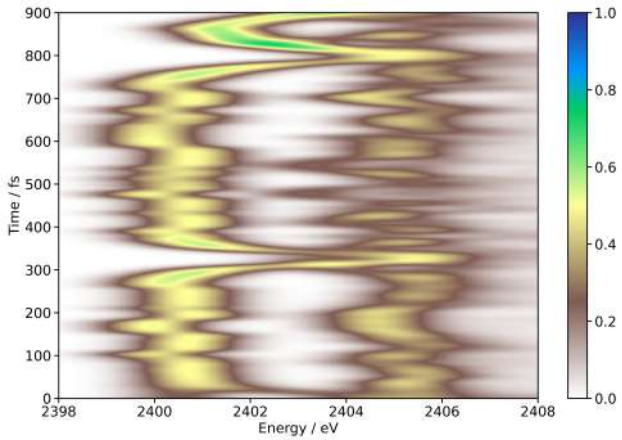

Figure S37: Trajectory 37: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

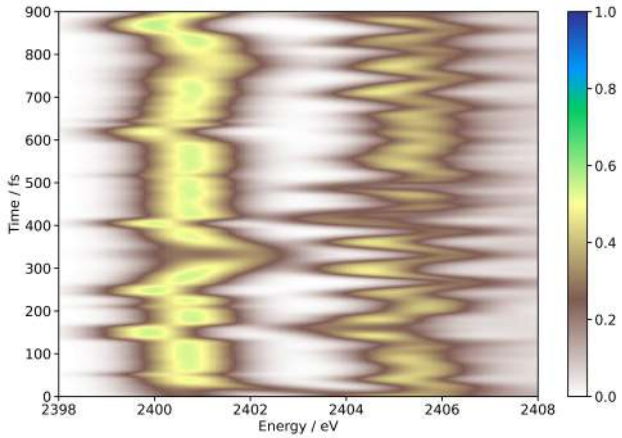

Figure S38: Trajectory 38: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

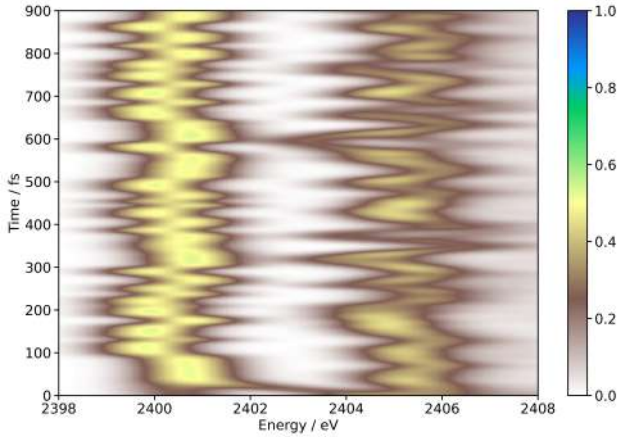

Figure S39: Trajectory 39: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

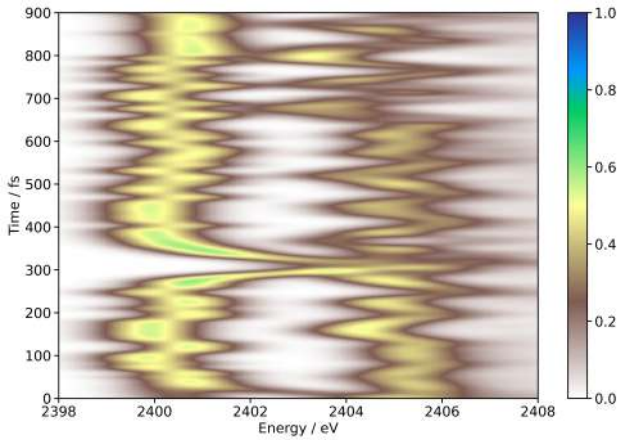

Figure S40: Trajectory 40: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

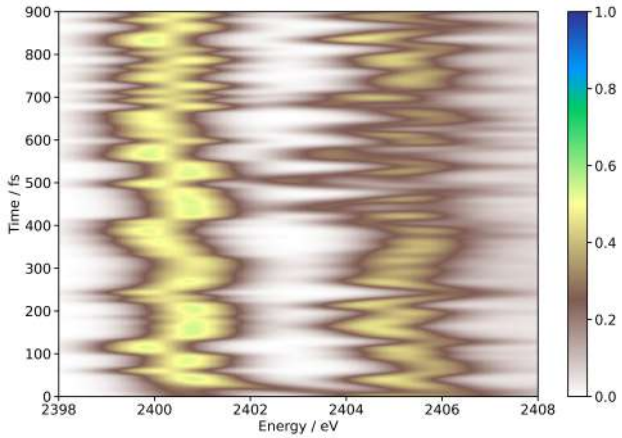

Figure S41: Trajectory 41: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

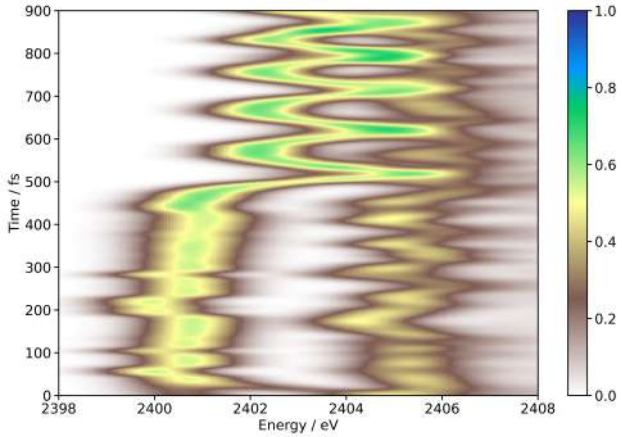

Figure S42: Trajectory 42: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

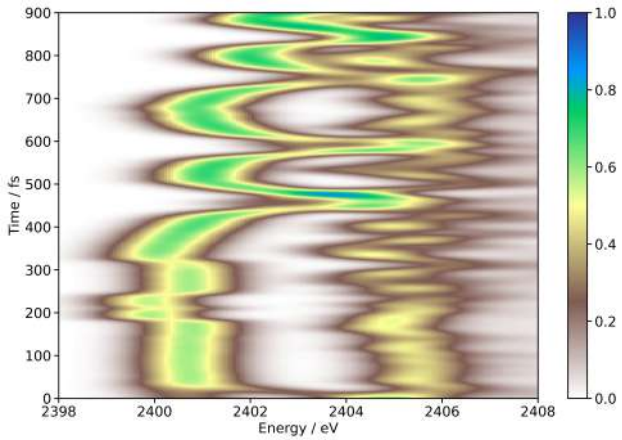

Figure S43: Trajectory 43: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

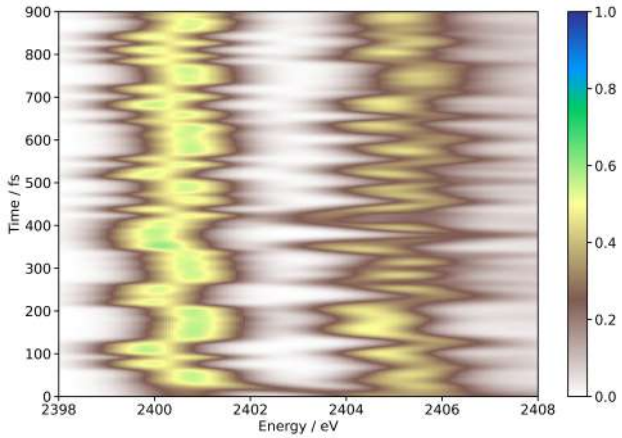

Figure S44: Trajectory 44: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

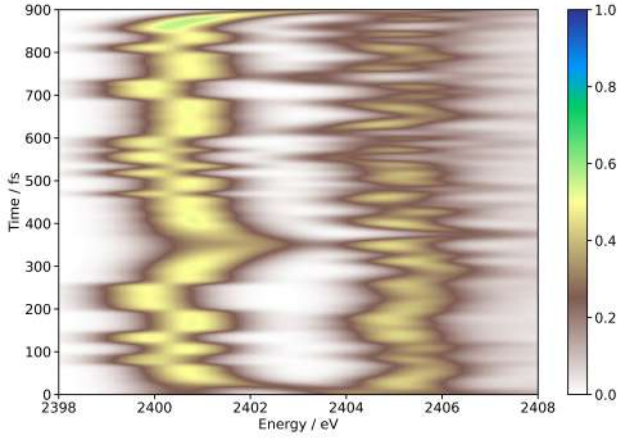

Figure S45: Trajectory 45: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

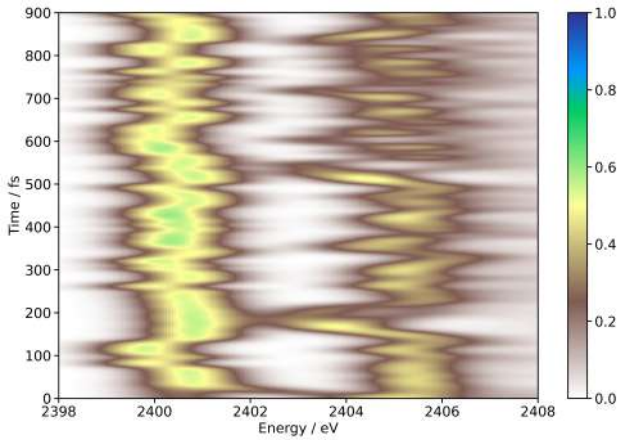

Figure S46: Trajectory 46: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

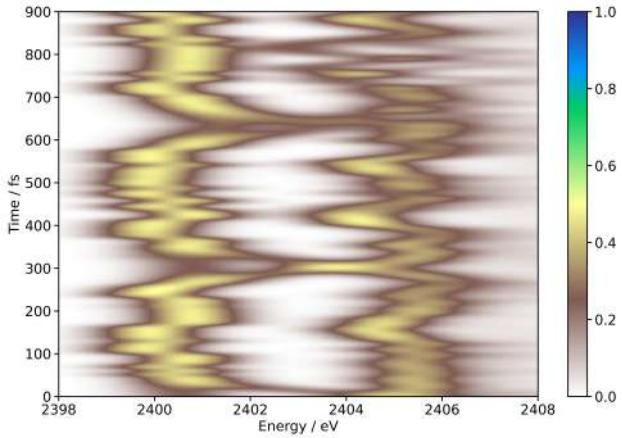

Figure S47: Trajectory 47: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

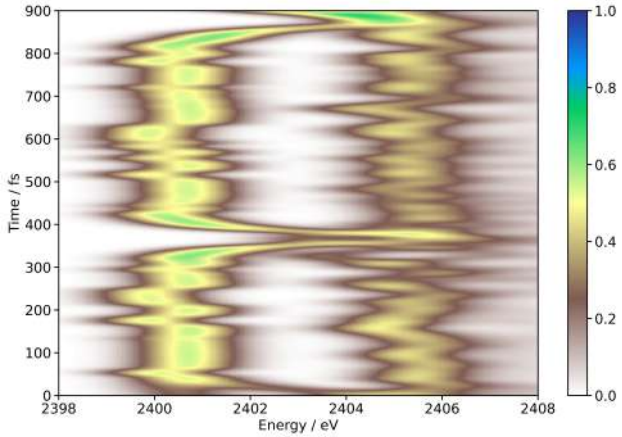

Figure S48: Trajectory 48: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

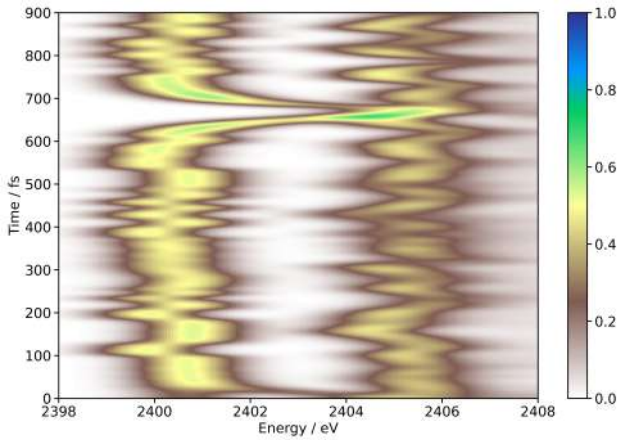

Figure S49: Trajectory 49: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

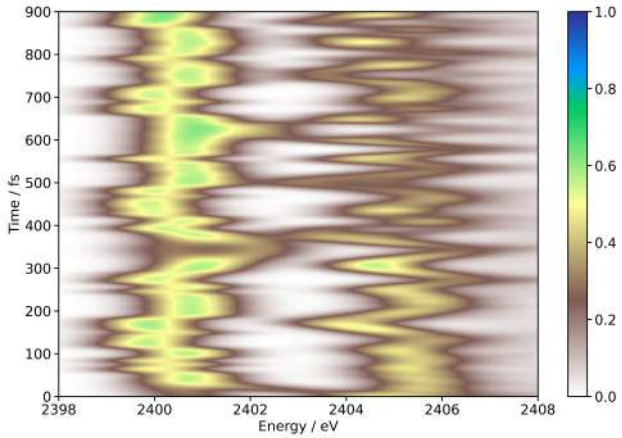

Figure S50: Trajectory 50: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

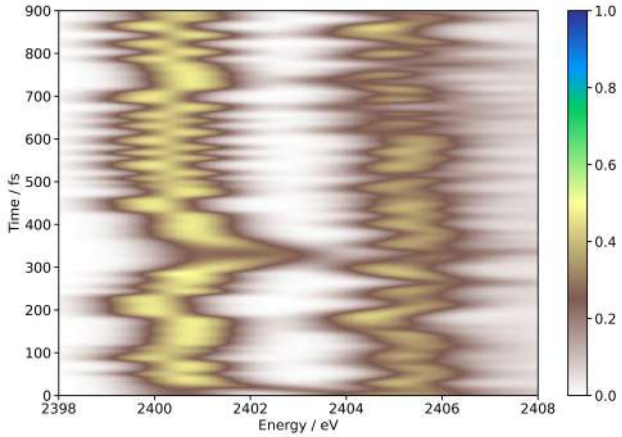

Figure S51: Trajectory 51: Time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated from first principles as described in the main text.

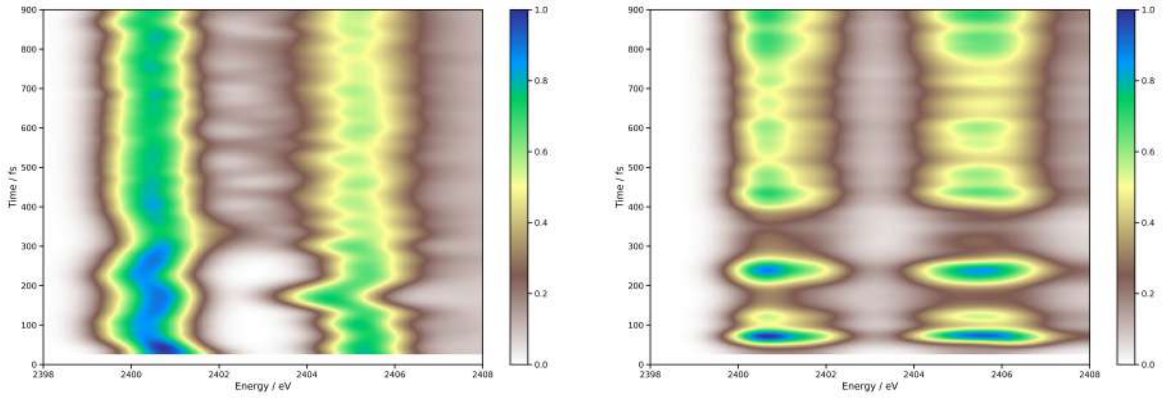

Figure S52: The time-resolved sulphur K-edge XAS spectra of the ring-opening dynamics of 1,2-dithiane calculated using DFT (a) and predicted using the DNN described in the main text (b). The plots are both shown from 30 fs, as this DNN has been trained on first principles data from all timesteps preceding 30 fs.

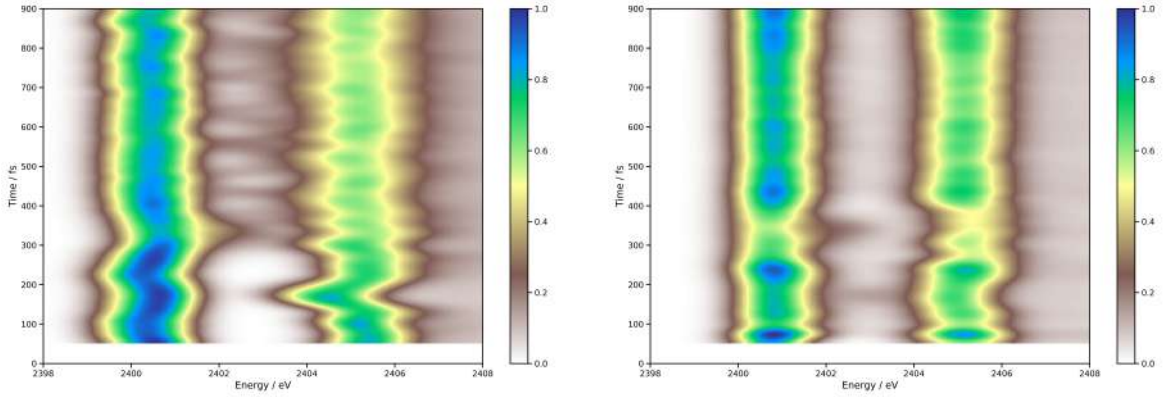

Figure S53: The time-resolved sulphur K-edge XAS spectra of the ring-opening dynamics of 1,2-dithiane calculated using DFT (a) and predicted using the DNN described in the main text (b). The plots are both shown from 60 fs, as this DNN has been trained on first principles data from all timesteps preceding 60 fs.

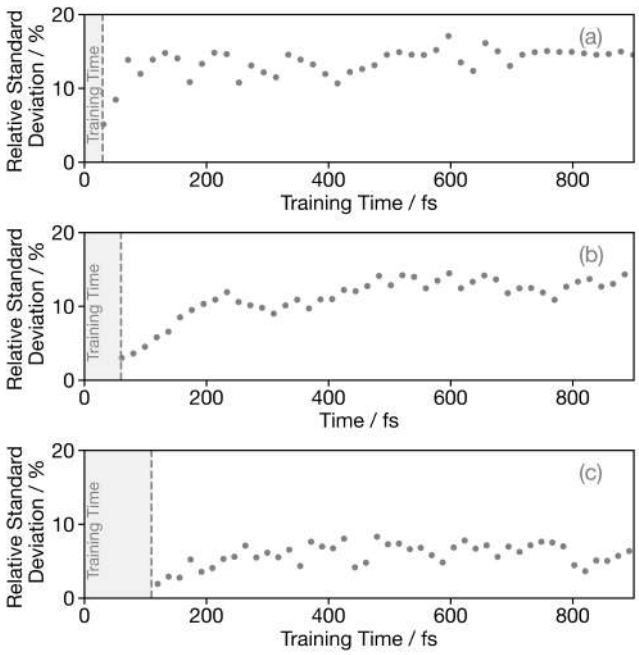

Figure S54: Median relative standard deviation as a function of time for the spectra trained up to (a) 30 fs, (b) 60 fs and (c) 110 fs.

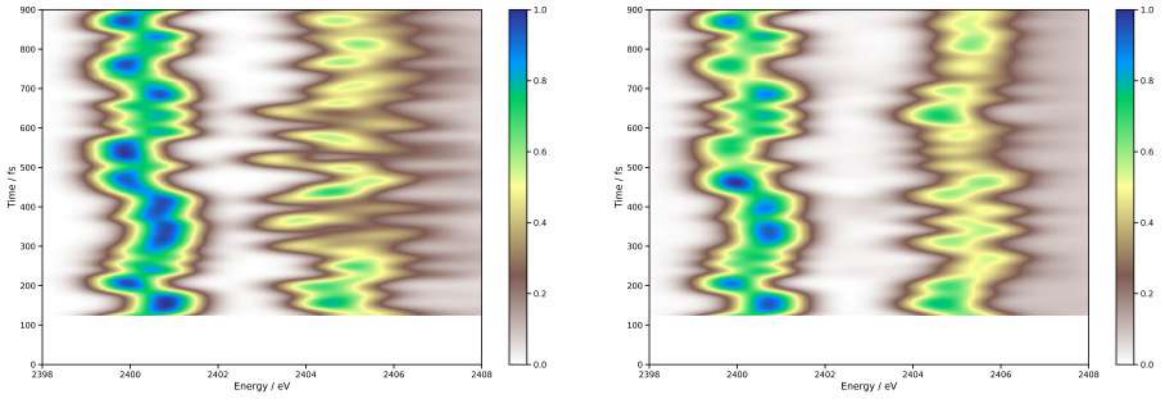

Figure S55: Trajectory 4: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 4) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

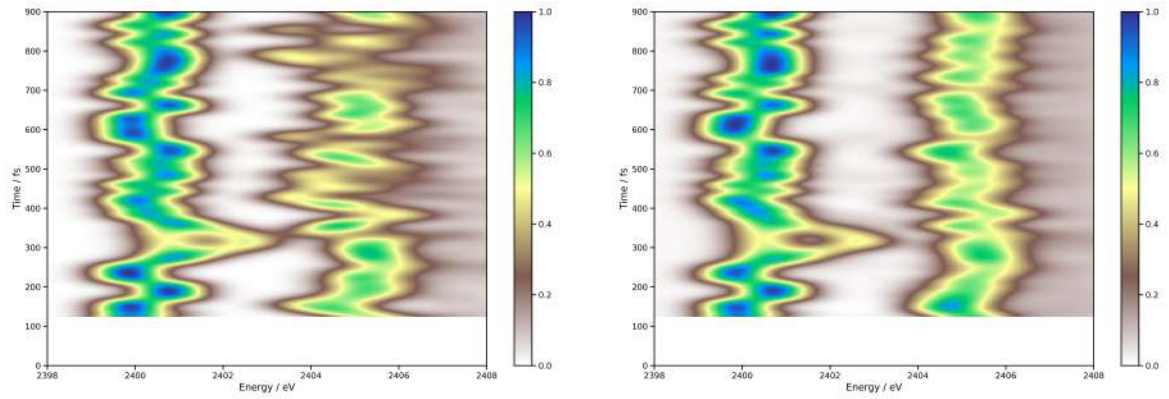

Figure S56: Trajectory 5: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 5) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

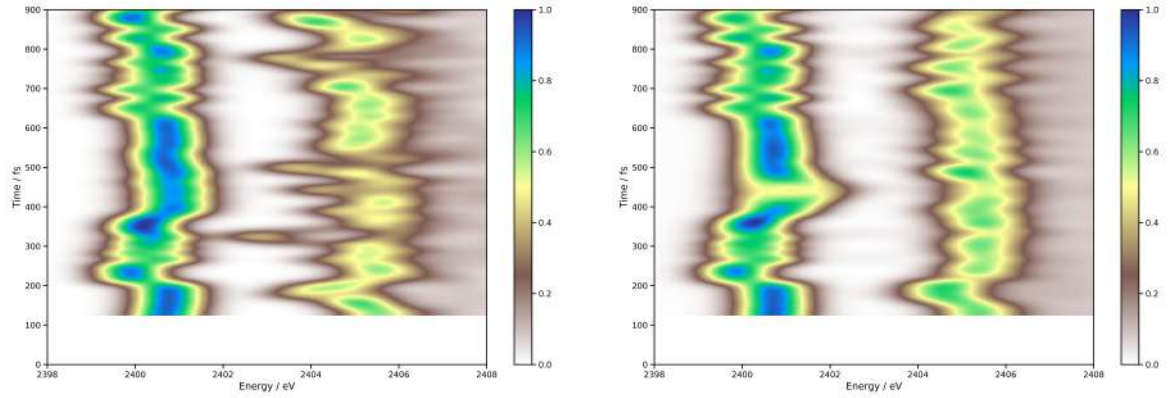

Figure S57: Trajectory 6: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 6) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

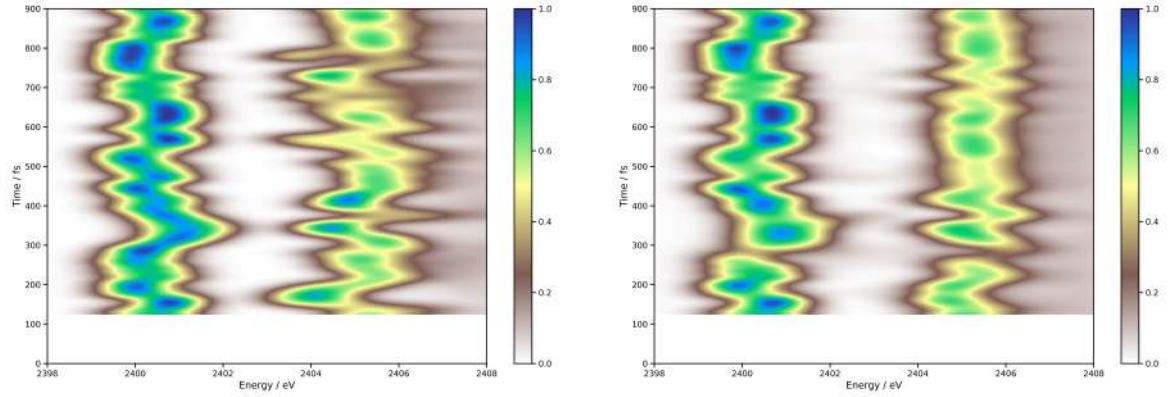

Figure S58: Trajectory 7: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 7) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

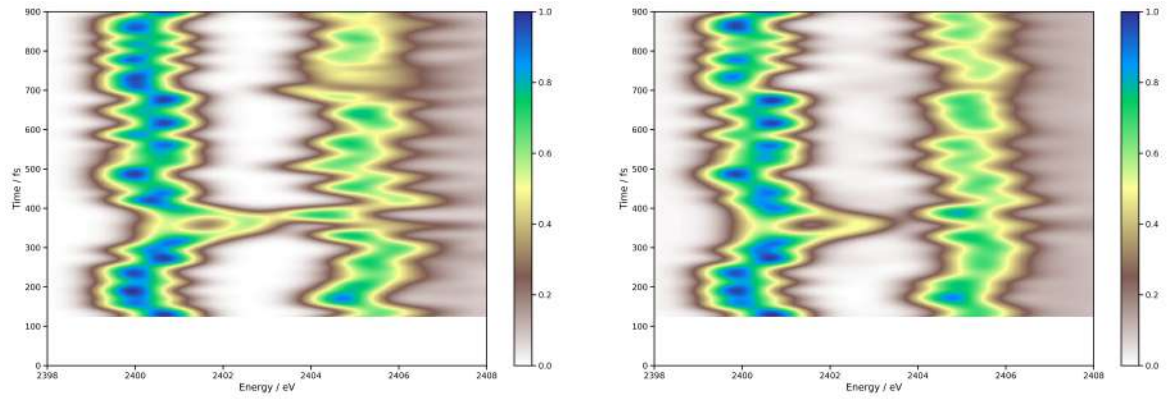

Figure S59: Trajectory 8: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 8) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

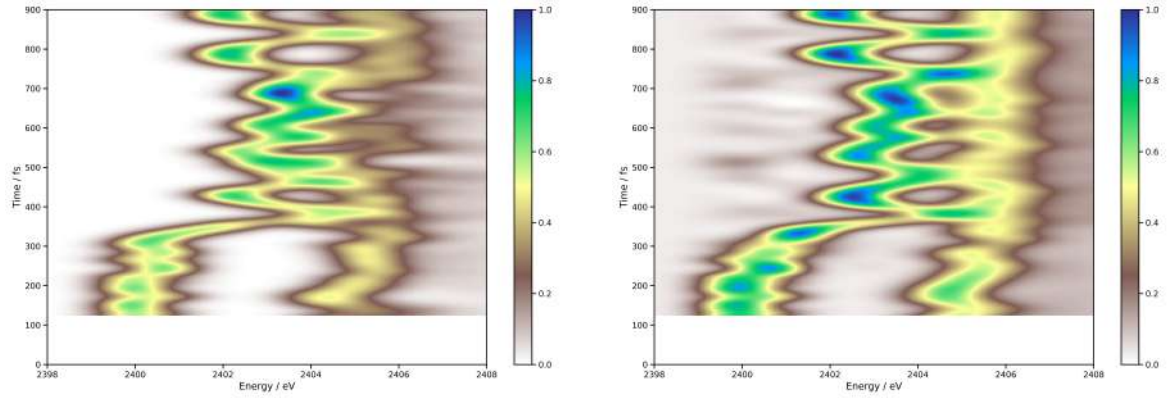

Figure S60: Trajectory 9: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 9) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

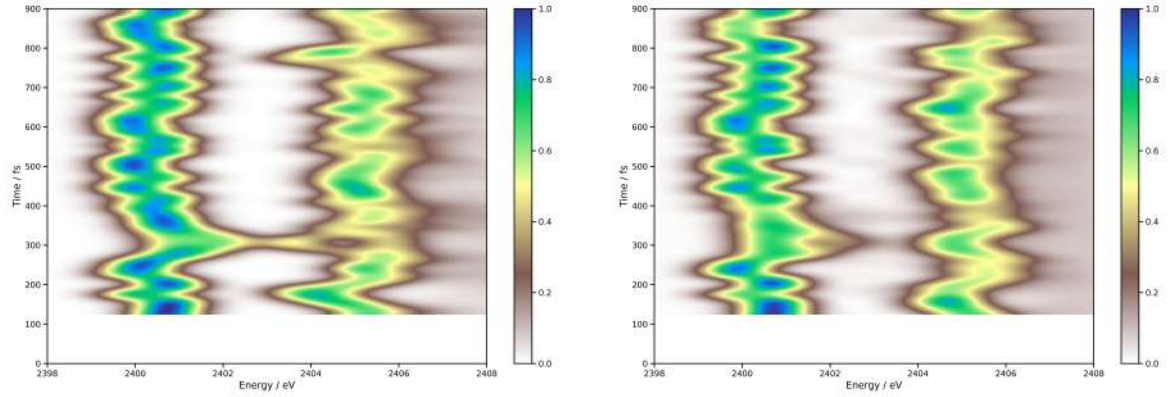

Figure S61: Trajectory 10: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 10) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

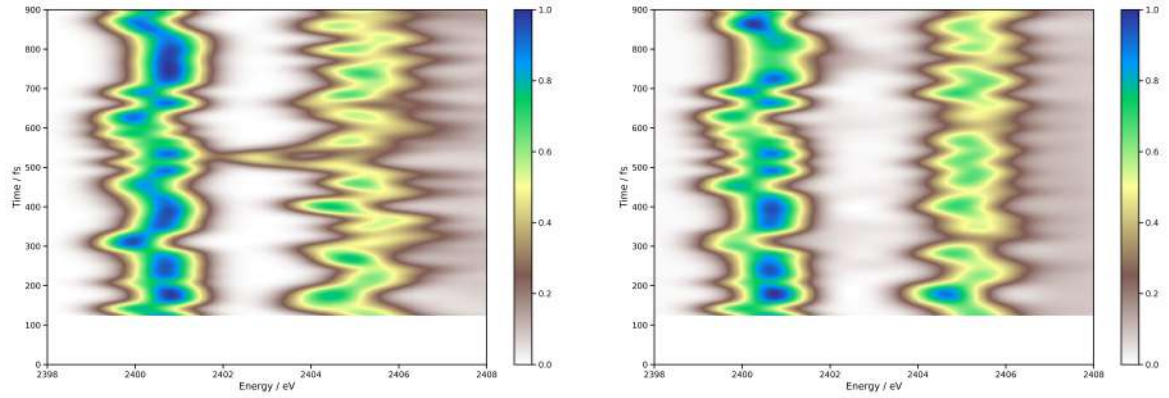

Figure S62: Trajectory 11: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 11) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

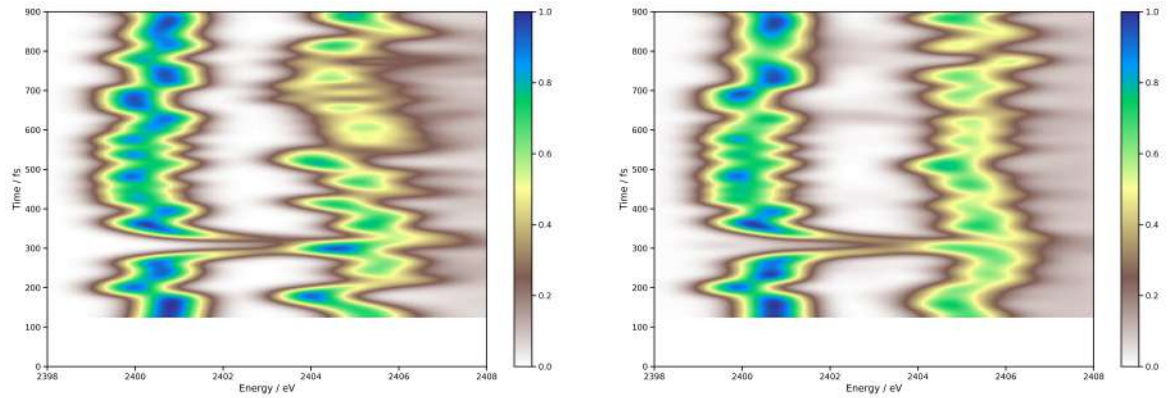

Figure S63: Trajectory 12: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 12) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

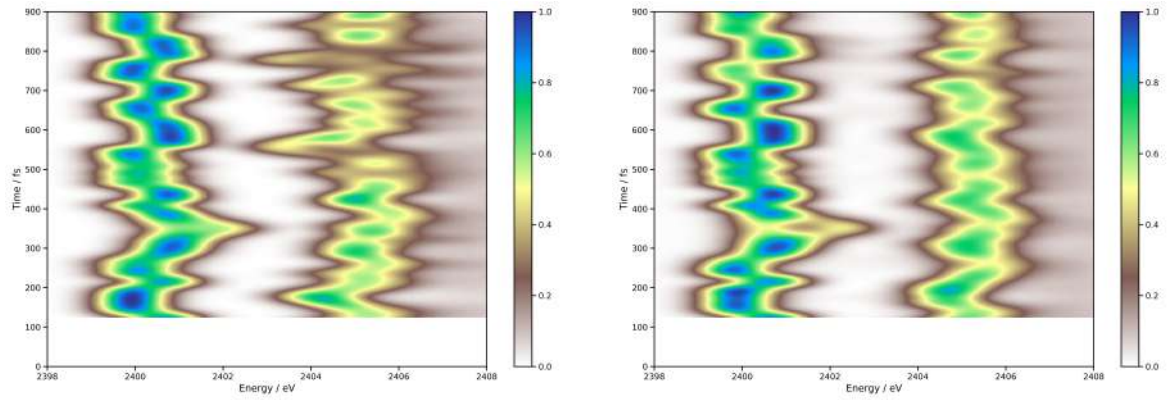

Figure S64: Trajectory 13: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 13) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs DFT.

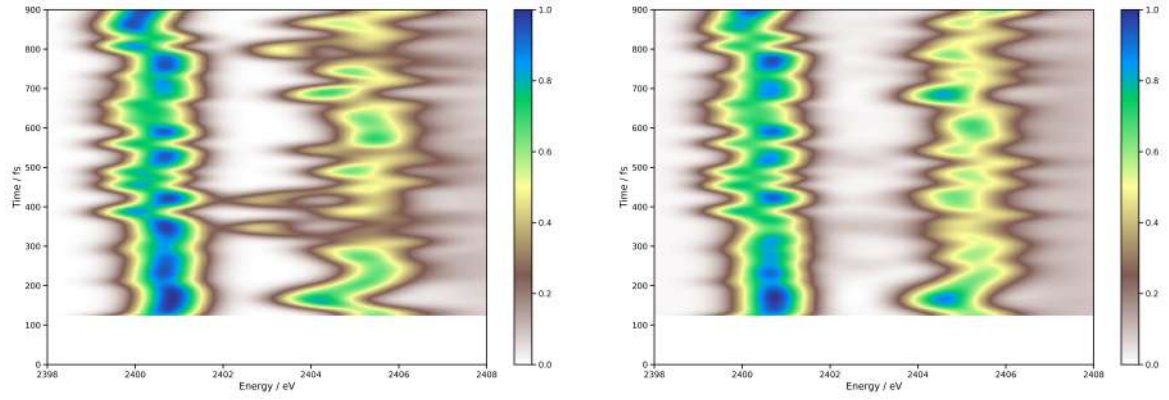

Figure S65: Trajectory 14: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 14) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

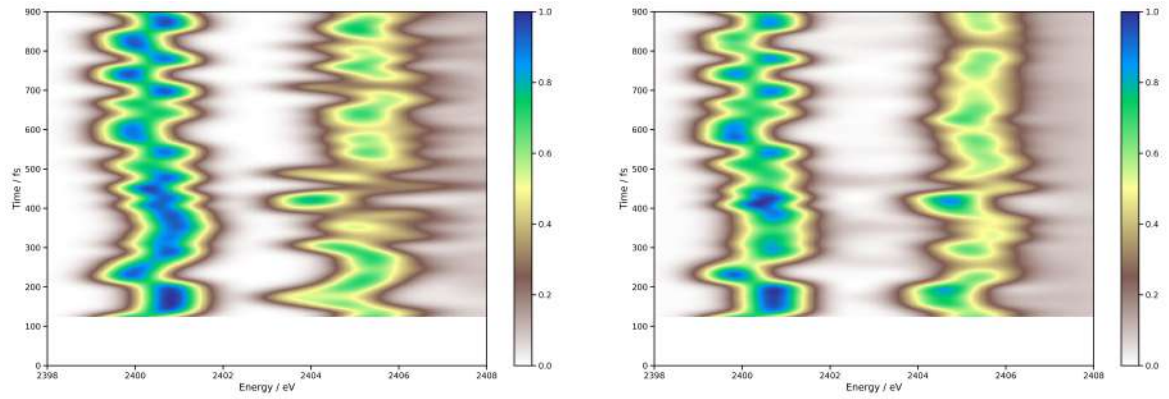

Figure S66: Trajectory 15: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 15) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

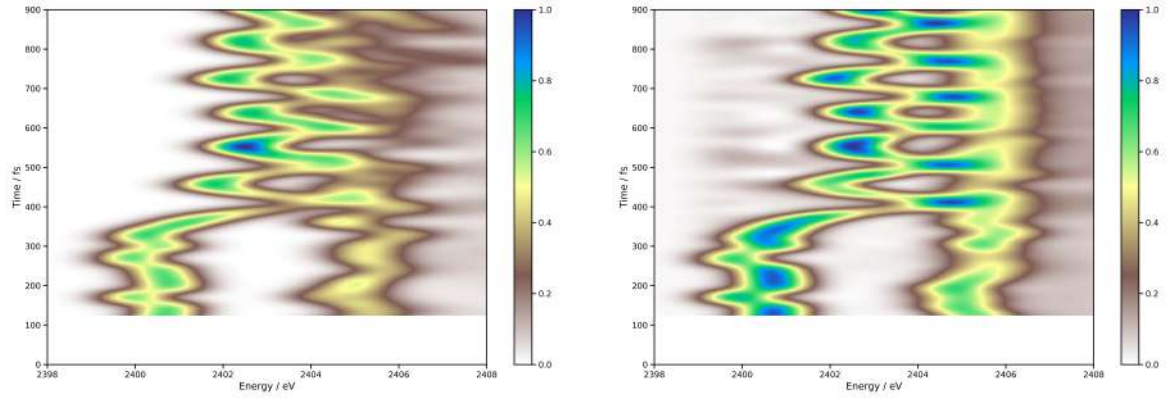

Figure S67: Trajectory 16: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 16) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

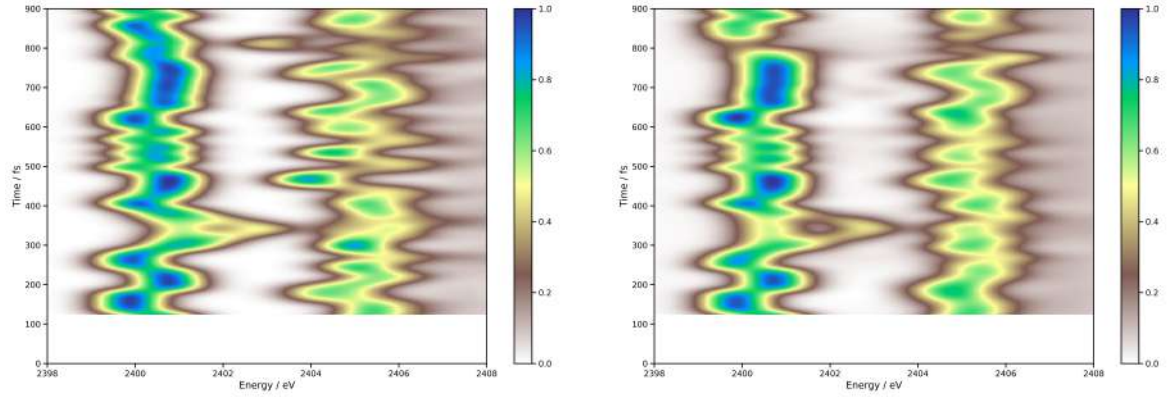

Figure S68: Trajectory 17: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 17) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

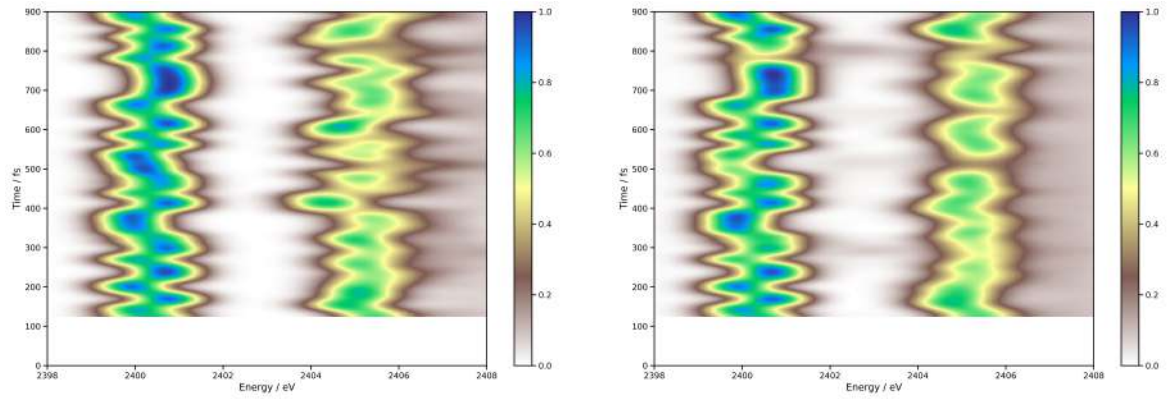

Figure S69: Trajectory 18: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 18) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

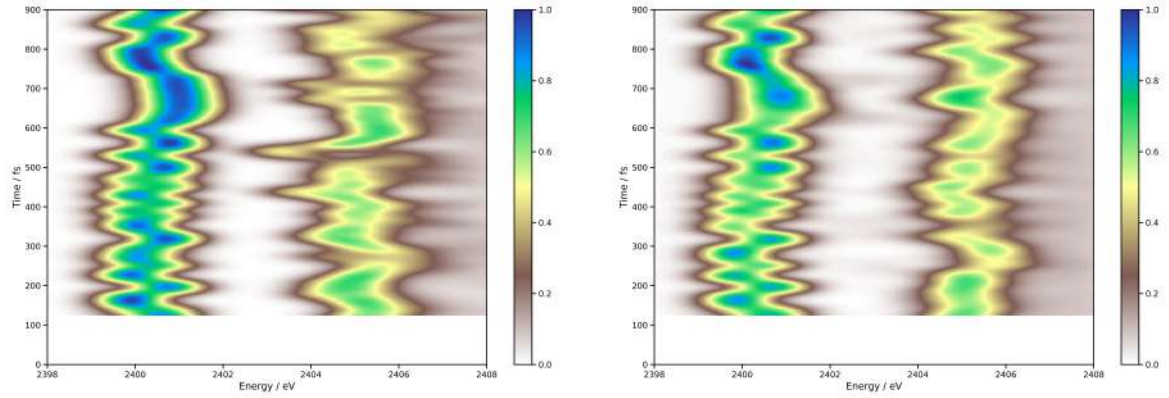

Figure S70: Trajectory 19: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 19) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

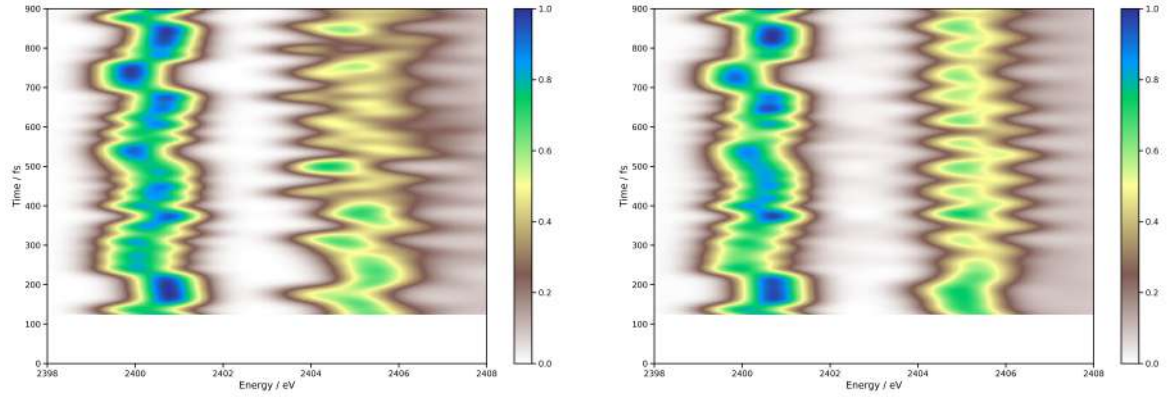

Figure S71: Trajectory 20: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 20) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

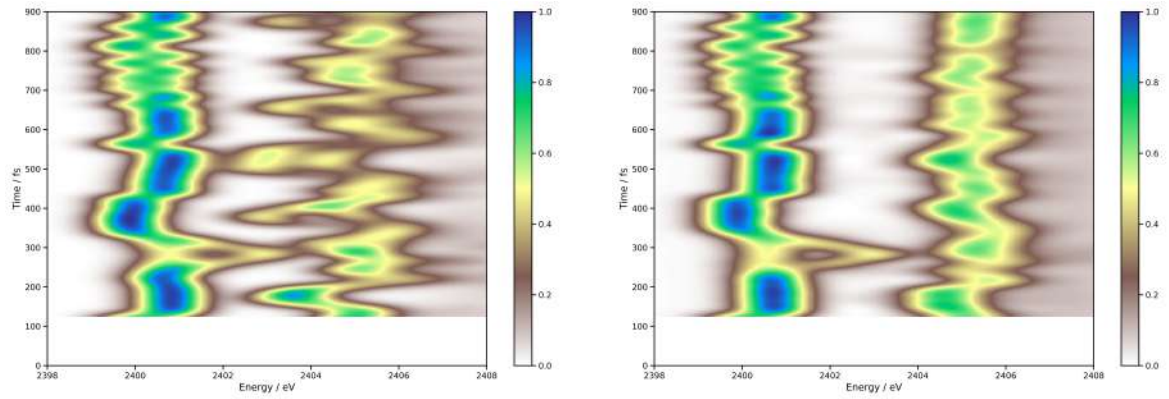

Figure S72: Trajectory 21: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 21) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

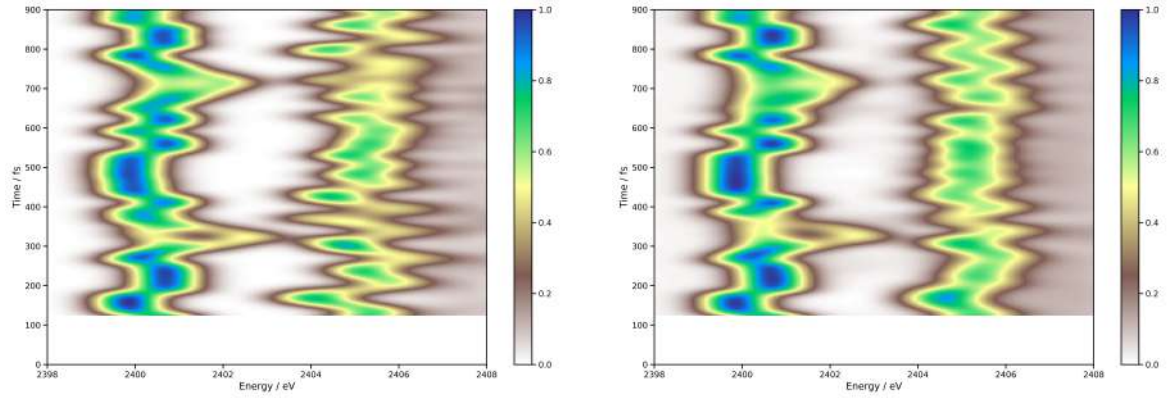

Figure S73: Trajectory 22: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 22) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

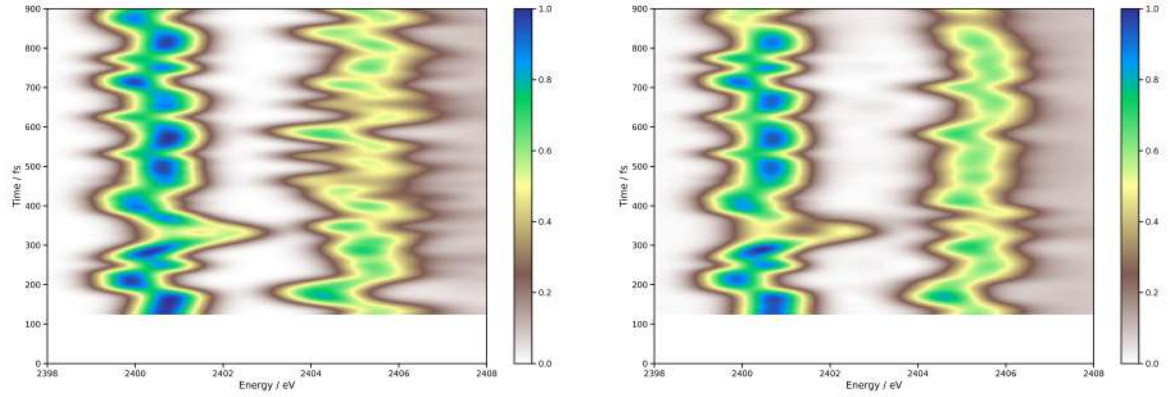

Figure S74: Trajectory 23: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 23) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

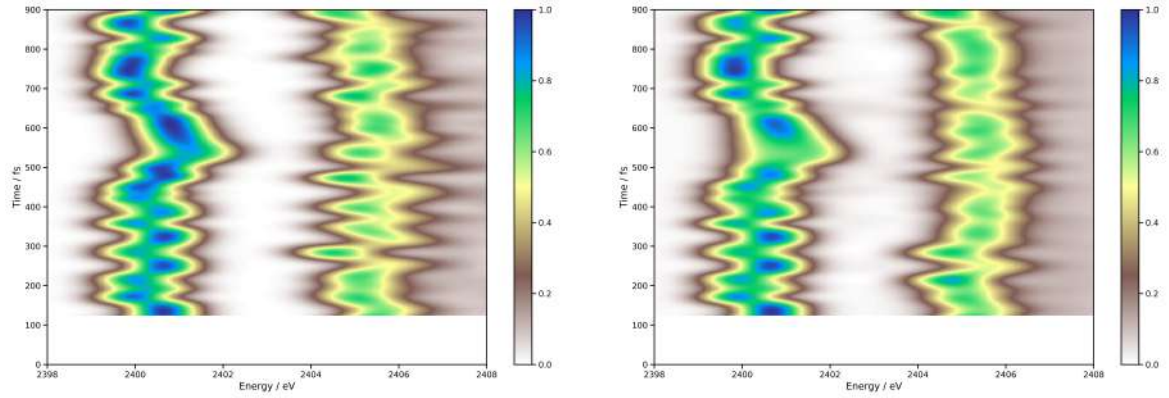

Figure S75: Trajectory 24: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 24) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

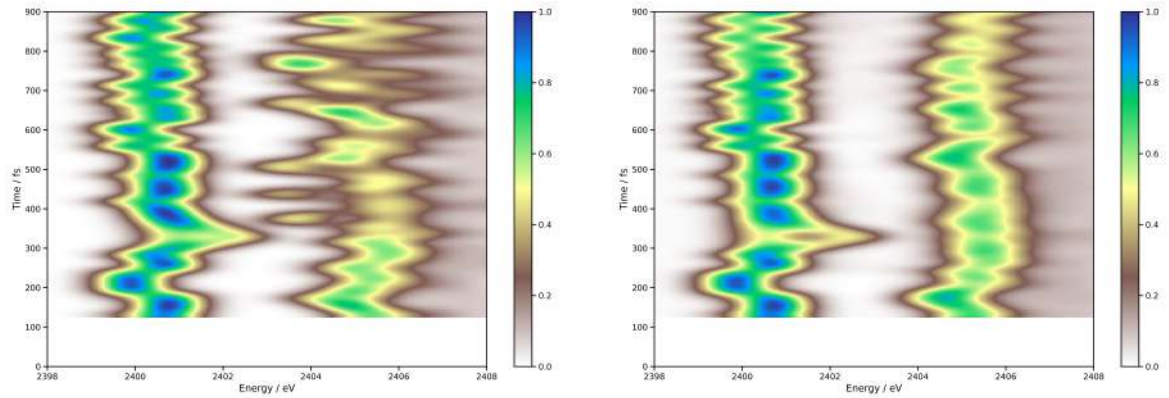

Figure S76: Trajectory 25: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 25) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

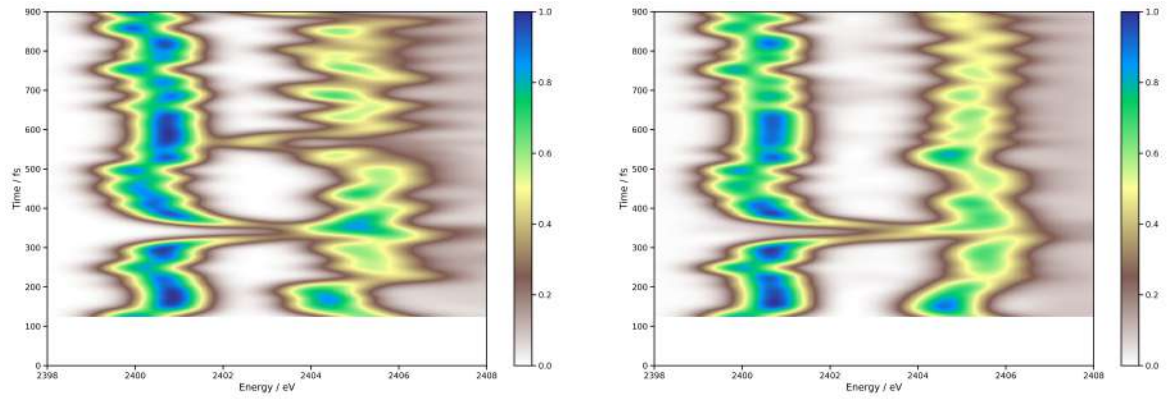

Figure S77: Trajectory 26: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 26) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

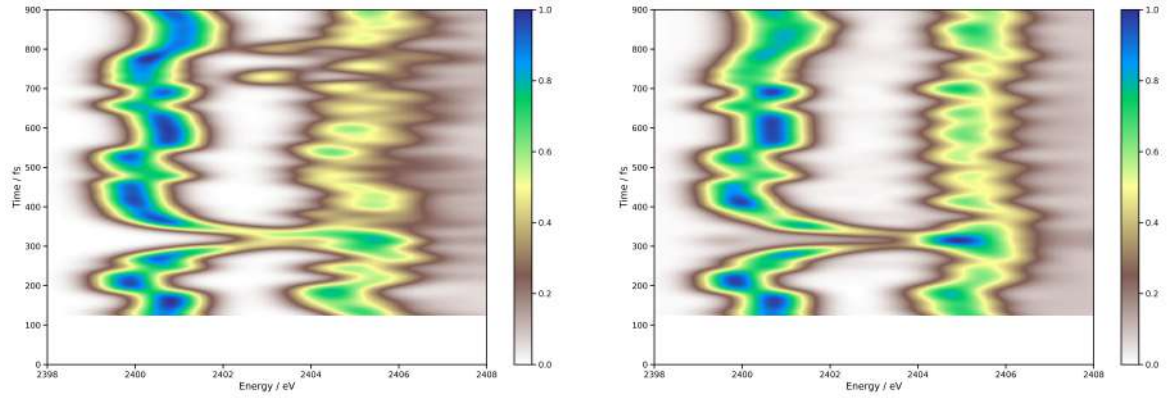

Figure S78: Trajectory 27: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 27) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

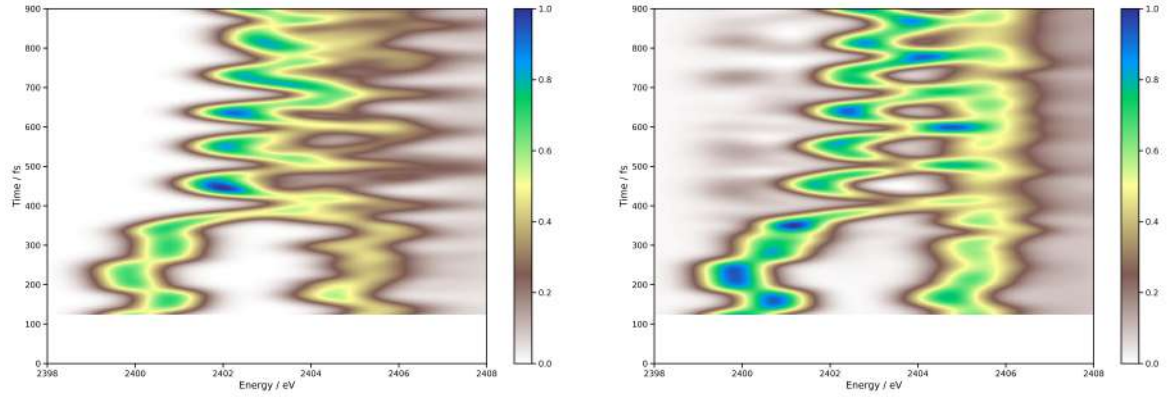

Figure S79: Trajectory 28: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 28) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

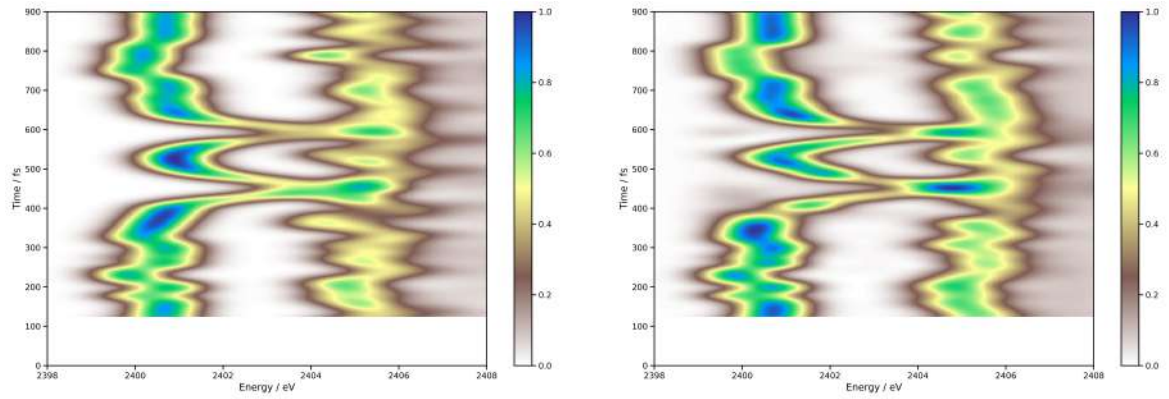

Figure S80: Trajectory 29: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 29) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

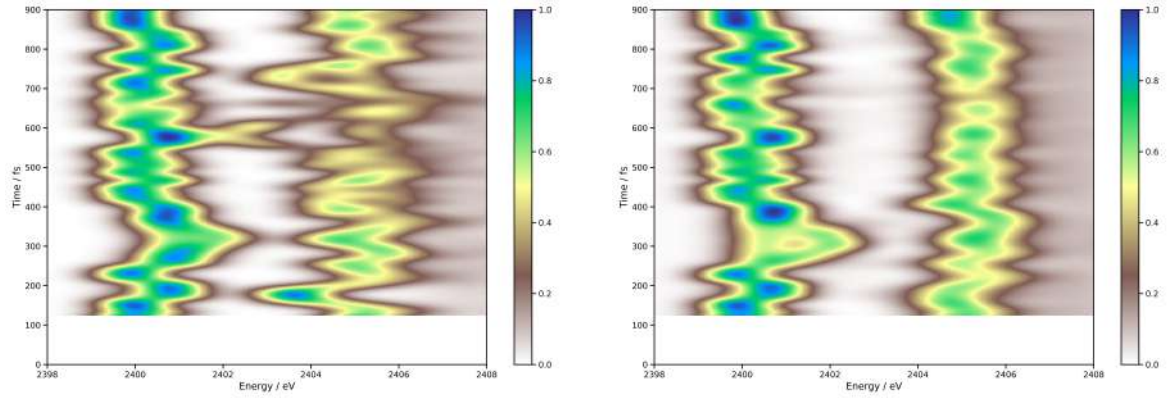

Figure S81: Trajectory 30: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 30) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

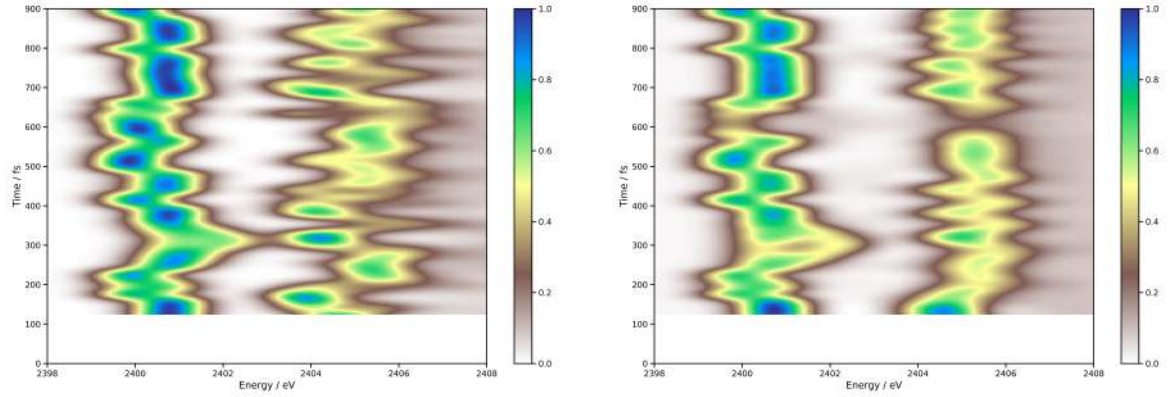

Figure S82: Trajectory 31: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 31) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

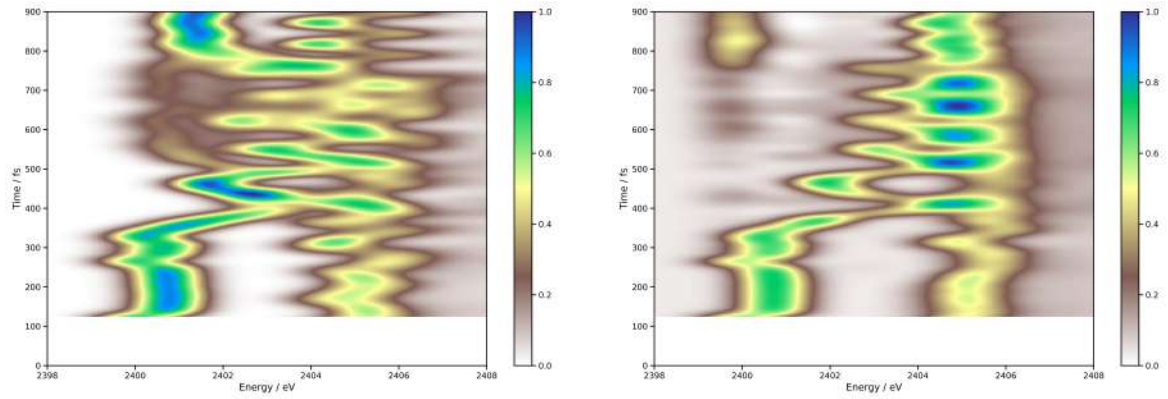

Figure S83: Trajectory 32: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 32) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

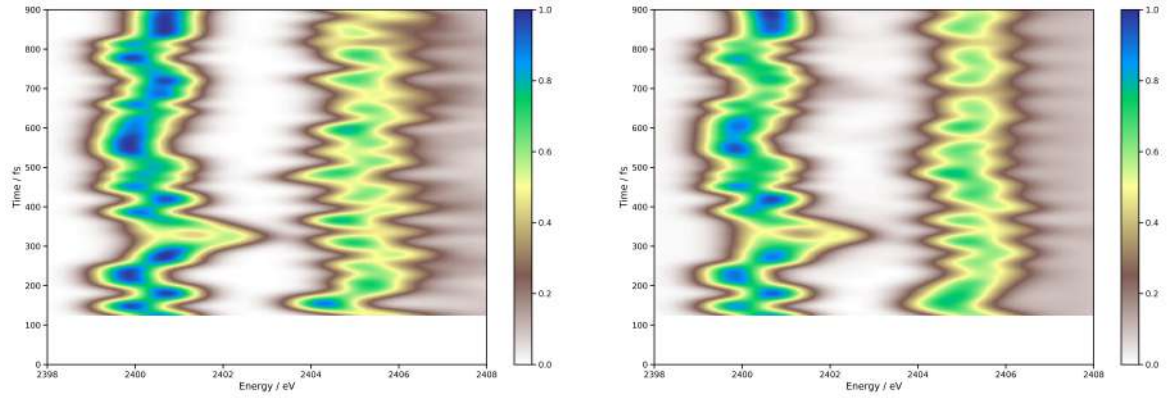

Figure S84: Trajectory 33: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 33) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

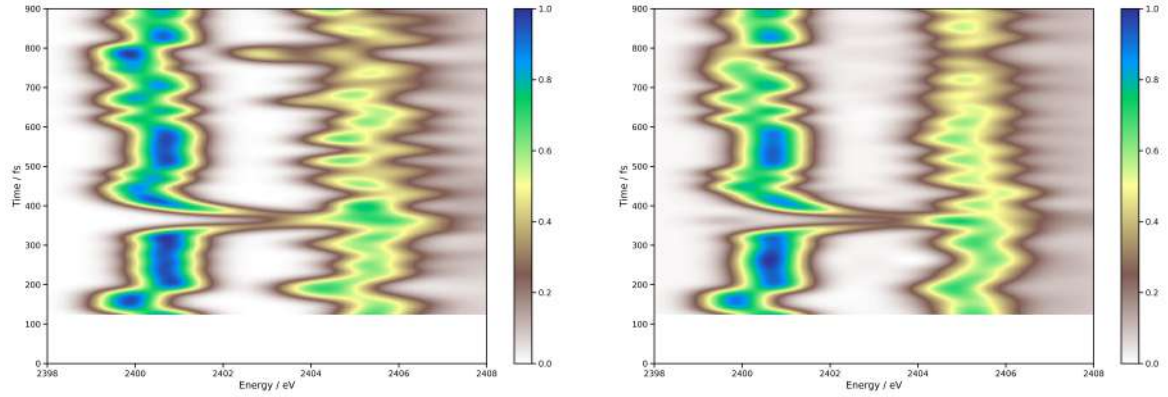

Figure S85: Trajectory 34: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 34) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

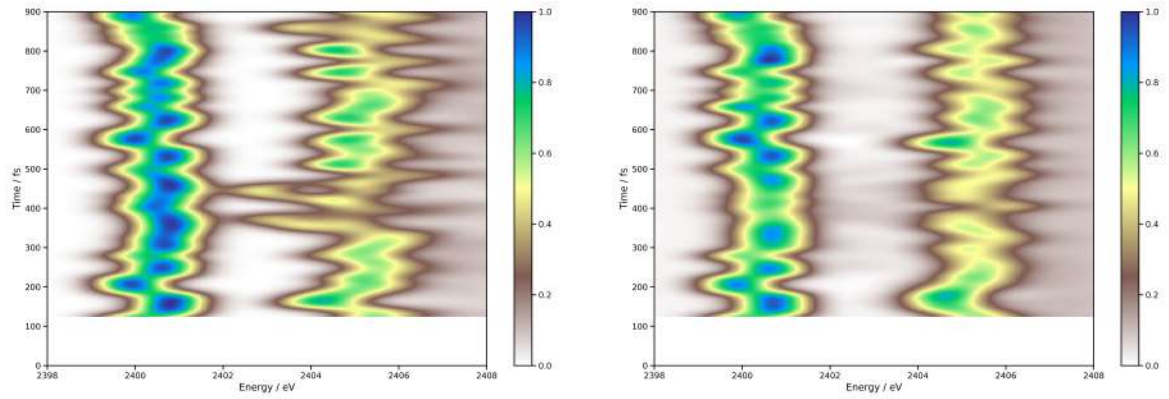

Figure S86: Trajectory 35: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 35) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

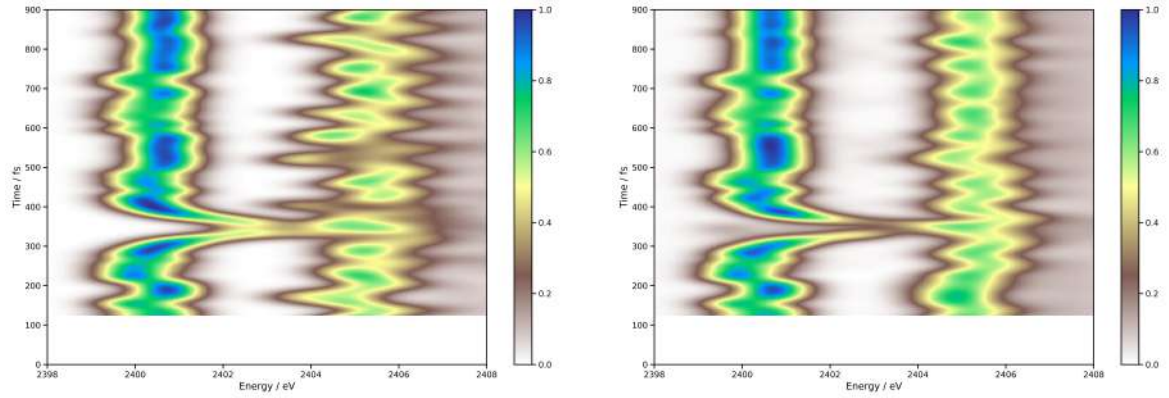

Figure S87: Trajectory 36: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 36) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

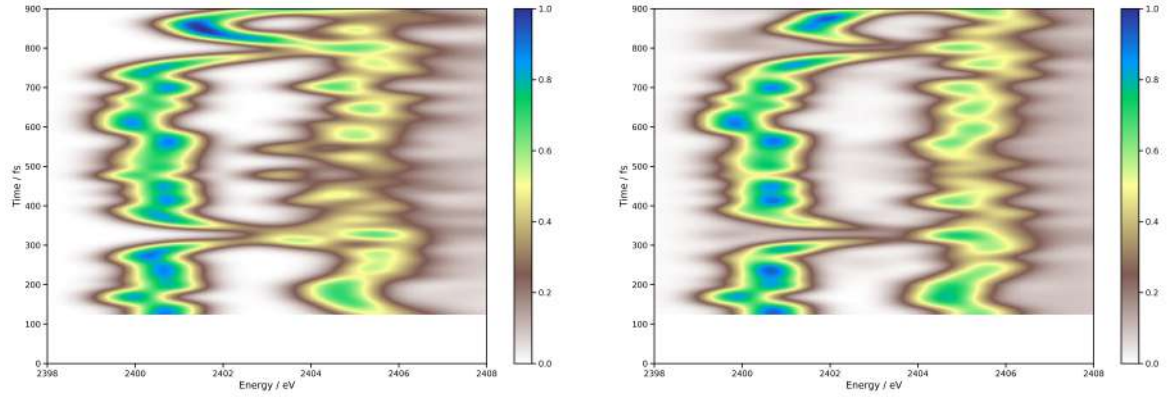

Figure S88: Trajectory 37: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 37) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

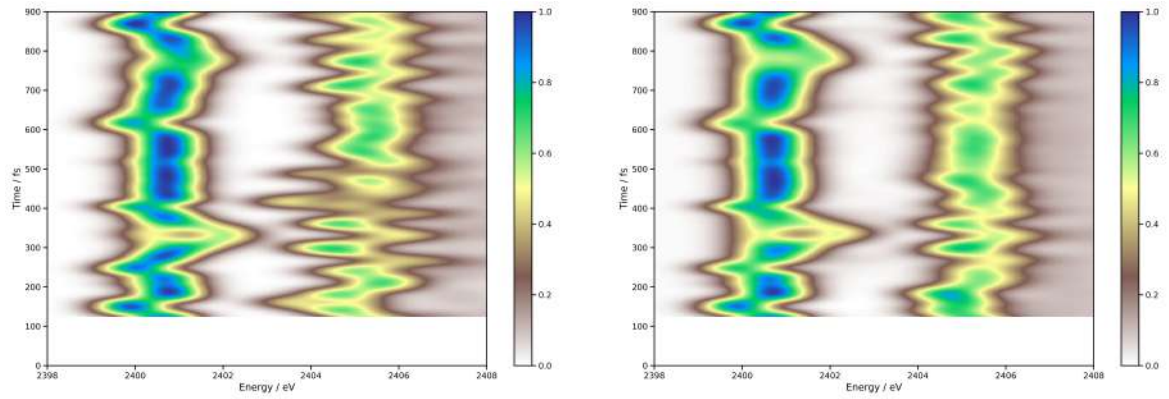

Figure S89: Trajectory 38: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 38) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

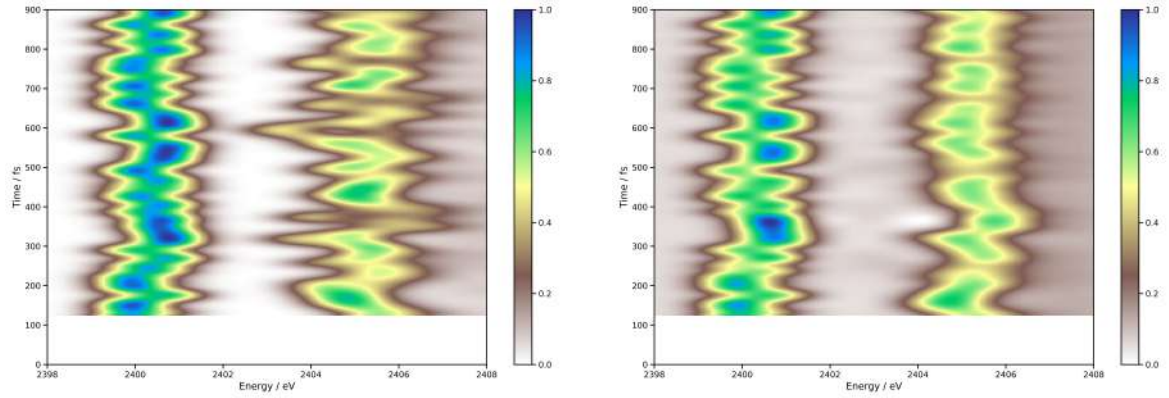

Figure S90: Trajectory 39: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 39) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

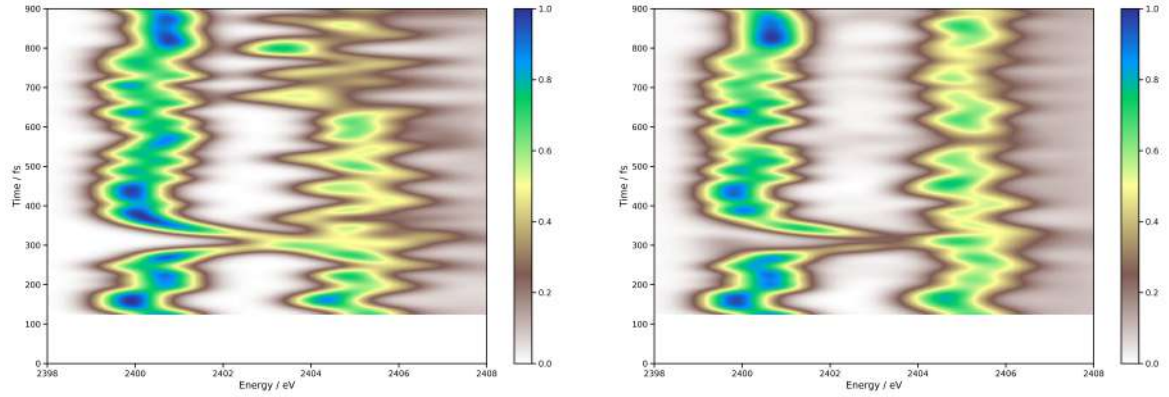

Figure S91: Trajectory 40: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 40) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

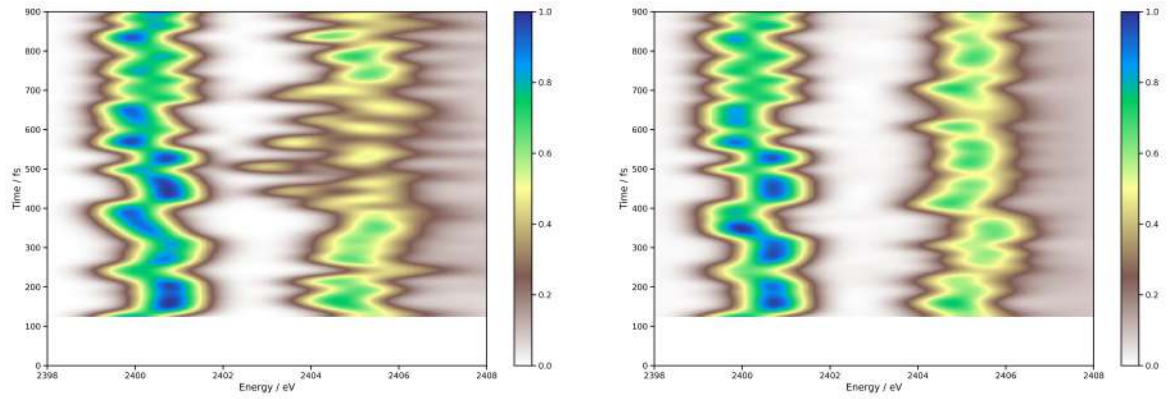

Figure S92: Trajectory 41: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 41) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

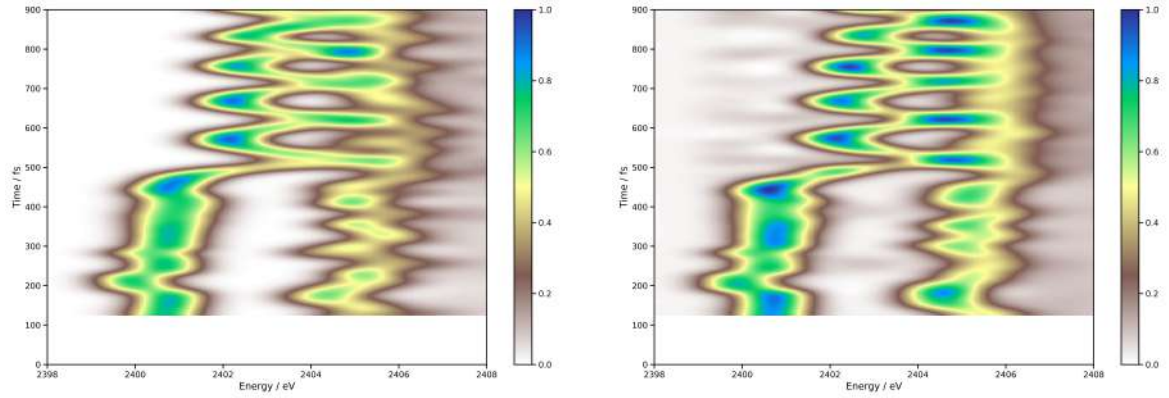

Figure S93: Trajectory 42: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 42) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

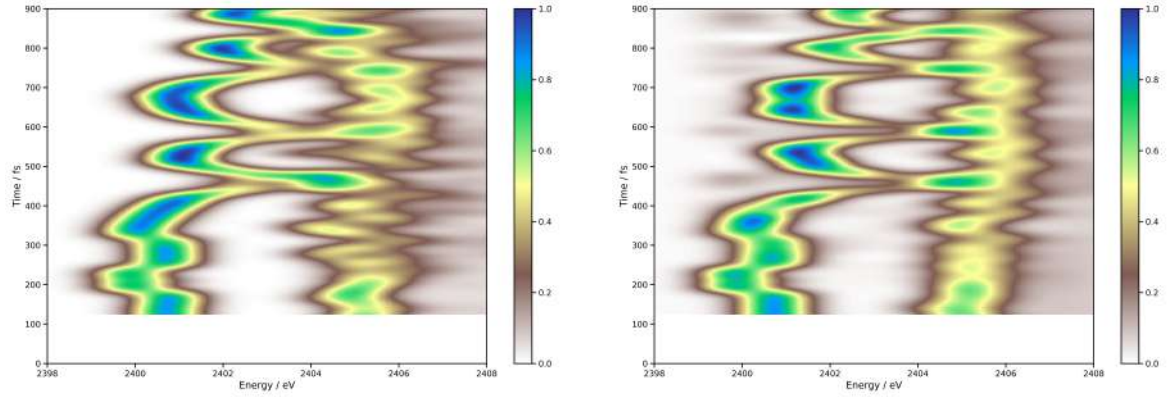

Figure S94: Trajectory 43: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 43) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

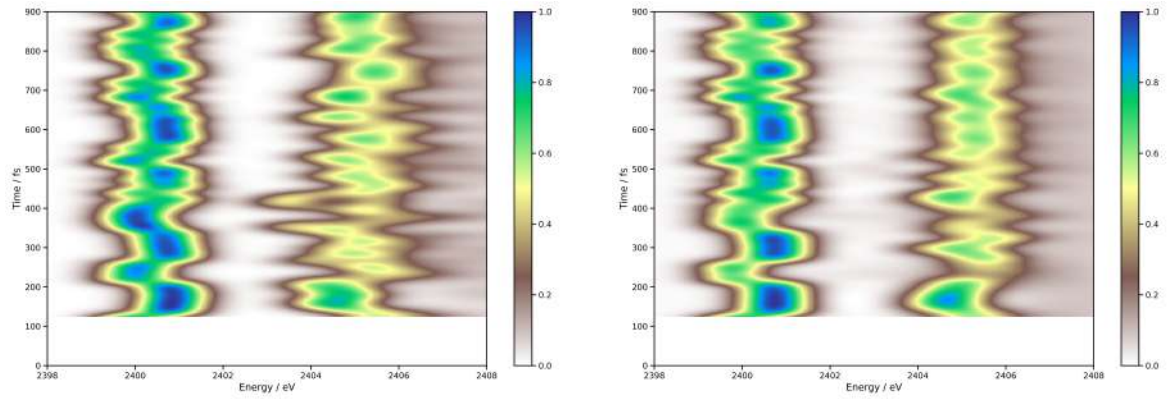

Figure S95: Trajectory 44: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 44) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

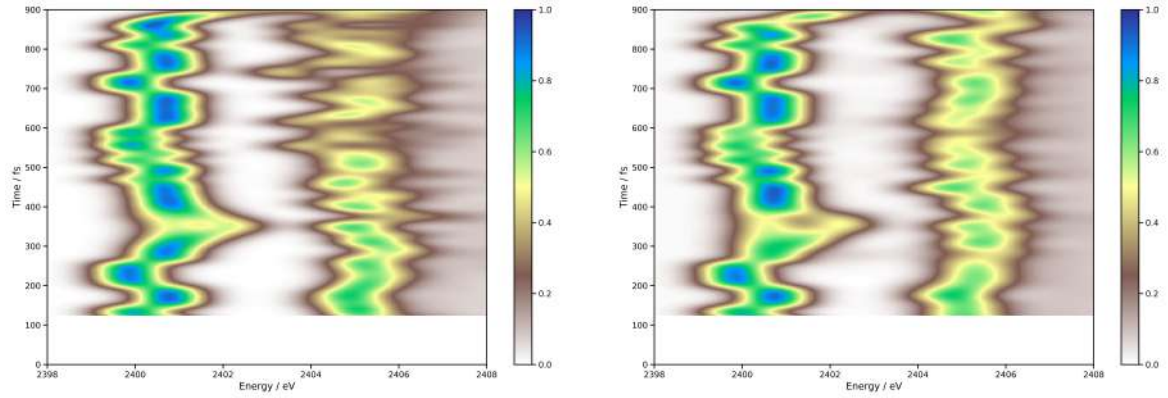

Figure S96: Trajectory 45: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 45) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

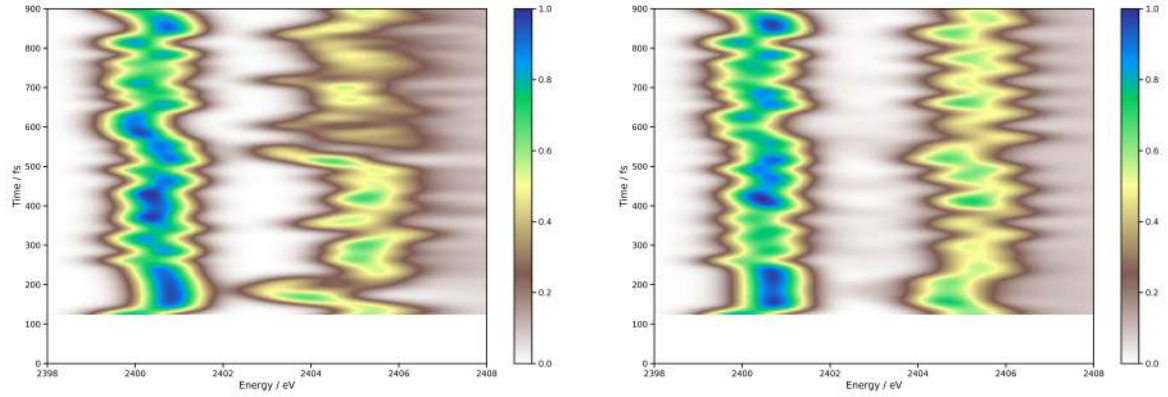

Figure S97: Trajectory 46: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 46) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

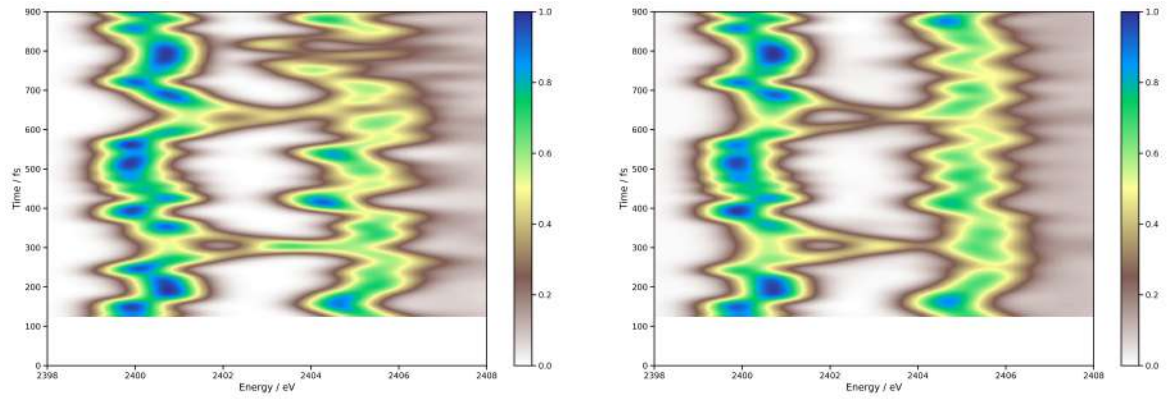

Figure S98: Trajectory 47: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 47) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

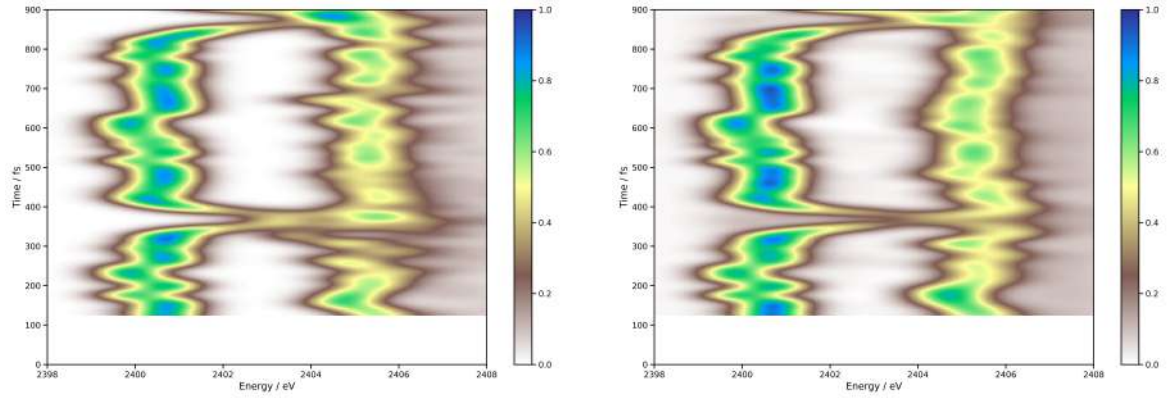

Figure S99: Trajectory 48: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 48) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

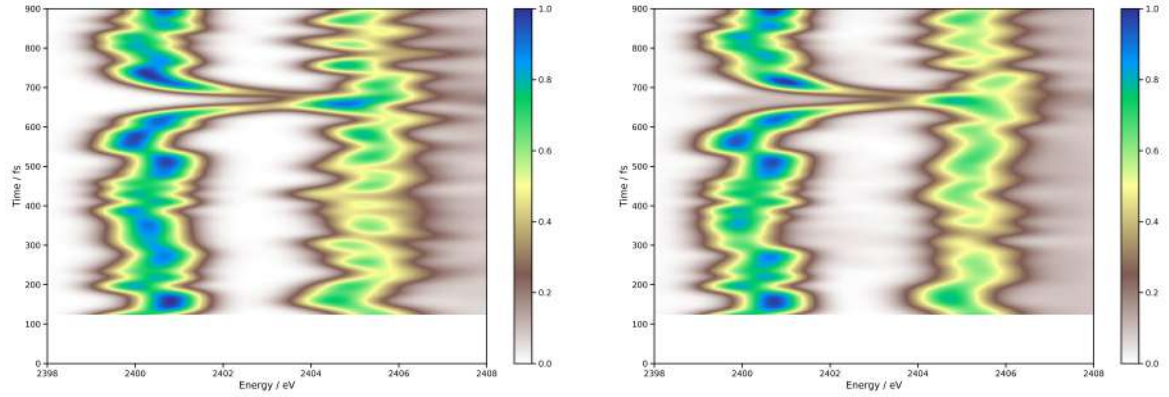

Figure S100: Trajectory 49: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 49) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

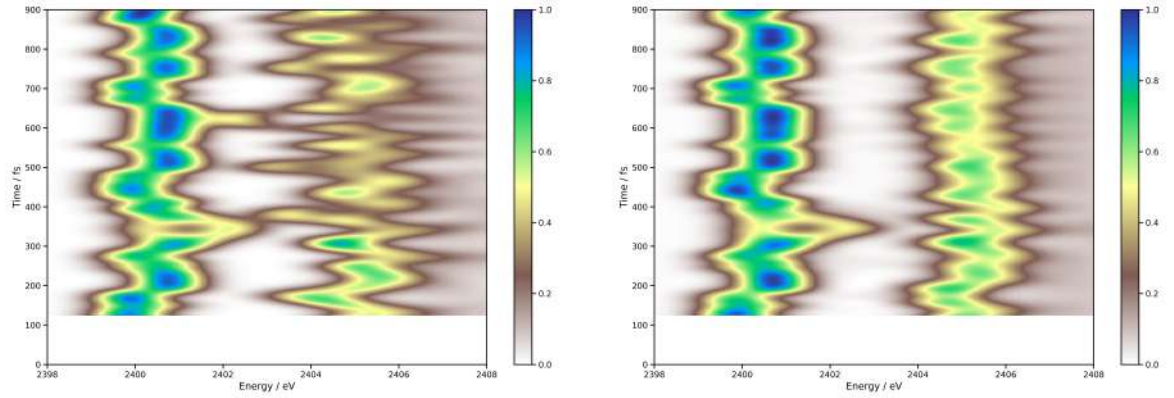

Figure S101: Trajectory 50: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 50) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.

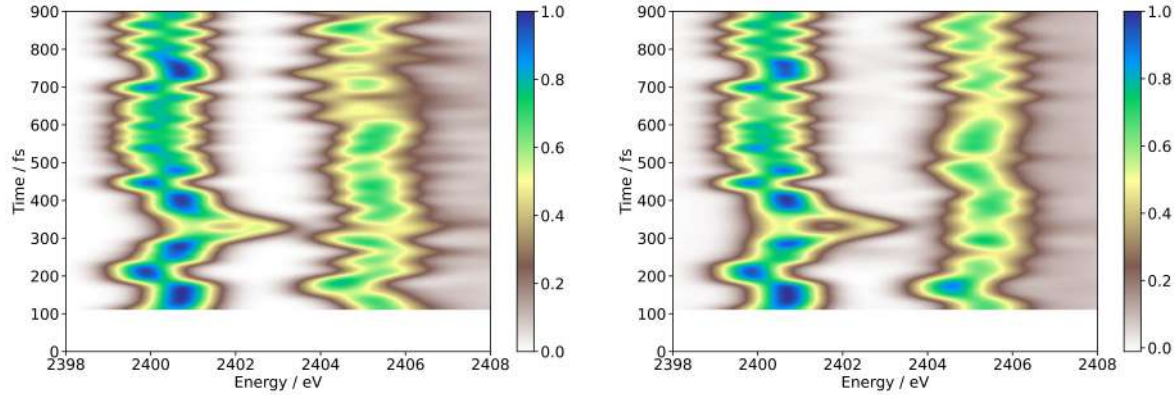

Figure S102: Trajectory 51: The time-resolved sulphur K-edge XAS of the ring-opening dynamics of 1,2-dithiane calculated using DFT (left) and predicted using the DNN described in the main text (right). These plots show the individual trajectories (trajectory 51) used in the ensemble. The plots are both shown from 120 fs, as the DNN is trained on first principles data from all timesteps preceding 110 fs.