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

Supplementary Information

Electron Paramagnetic Resonance and Microstructural Insights into the Thermal Behavior of Simonkolleite Nanoplatelets

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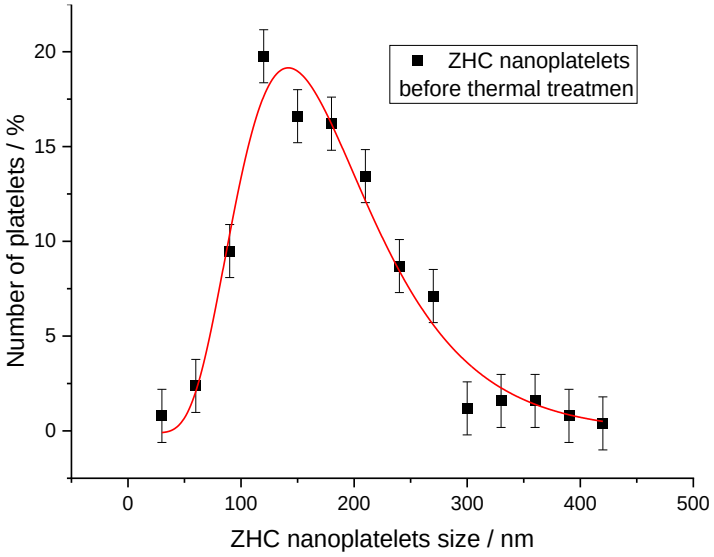

Figure S1. Particle size distributions for as-prepared ZHC sample.

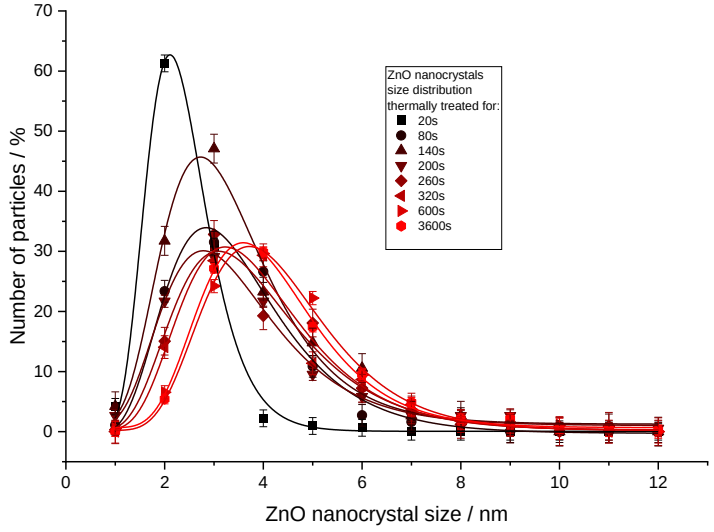

Figure S2. Particle size distributions of the thermally treated ZHC samples.

The fit function used was a Lognormal-function (Equation E1). The fit parameters for the different annealing times are depicted in Table 1.

$$y = y_0 + \frac{A}{\sqrt{2\pi}wx} e^{\frac{-\left[ln\frac{x}{x_c}\right]^2}{2w^2}}$$

Equation E1. Log-Normal function, which was used to fit the nanocrystal size distribution.

Table S1. The lognormal fit function parameters for the different annealing times.

	y0		xc		w		A		mu		sigma		Statistics	
	Value	Std. Error	Value	Std. Error	Value	Std. Error	Value	Std. Error	Value	Std. Error	Value	Std. Error	Reduced Chi-Sqr	Adj. R-Square
20s	0.05242	0.50317	68.73016	0.89002	0.28756	0.01871	2977.79519	102.53086	71.63149	0.75038	21.03194	1.3859	0.95934	0.99469
80s	0.28416	0.85458	99.50898	2.54678	0.39292	0.02745	3104.7826	159.64064	107.49454	3.5381	43.92033	4.51646	1.05308	0.97578
140s	1.24656	1.1816	94.38494	2.6431	0.37744	0.03118	3695.80028	222.22252	101.35316	3.61715	39.65823	4.66921	1.27708	0.96817
200s	1.01254	0.46535	98.05451	1.62449	0.3999	0.01829	2639.06267	86.04038	106.21697	2.29141	44.23245	2.98929	0.98318	0.99024
260s	0.16999	1.21508	108.22995	4.20503	0.39221	0.03922	2940.29713	229.12733	116.88292	5.76966	47.66354	7.10735	1.19195	0.94404
320s	0.25471	0.93376	110.81444	3.0922	0.36744	0.02753	2907.419	176.96805	118.55353	4.07123	45.07437	4.84975	1.12445	0.96469
600s	0.20759	0.5106	123.85405	1.55715	0.32473	0.01404	2926.41336	94.02524	130.55956	1.98471	43.53963	2.47979	0.9676	0.98989
3600s	0.66142	0.35567	119.1221	1.07145	0.31608	0.00995	2762.62421	65.57388	125.22386	1.33922	40.59057	1.65572	0.97826	0.99451

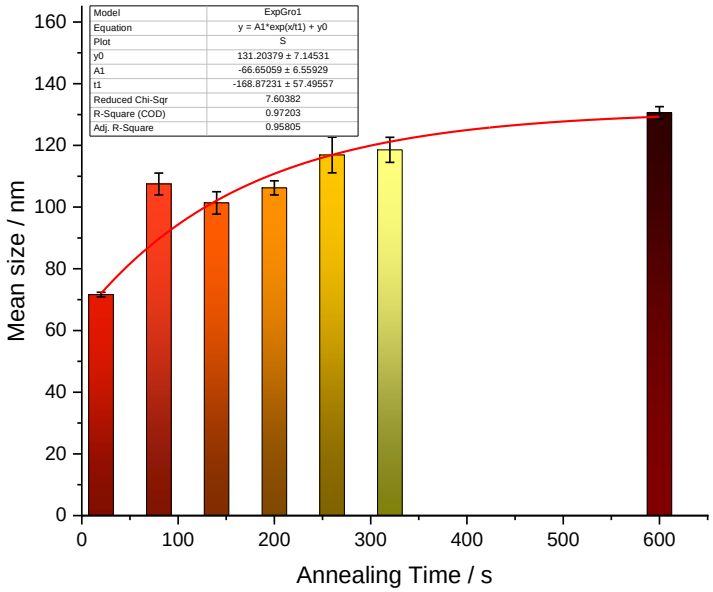

Figure S3. Growth rate of the nanocrystals mean size obtained from the size distribution fit of the nanoparticles sizes measured by TEM.

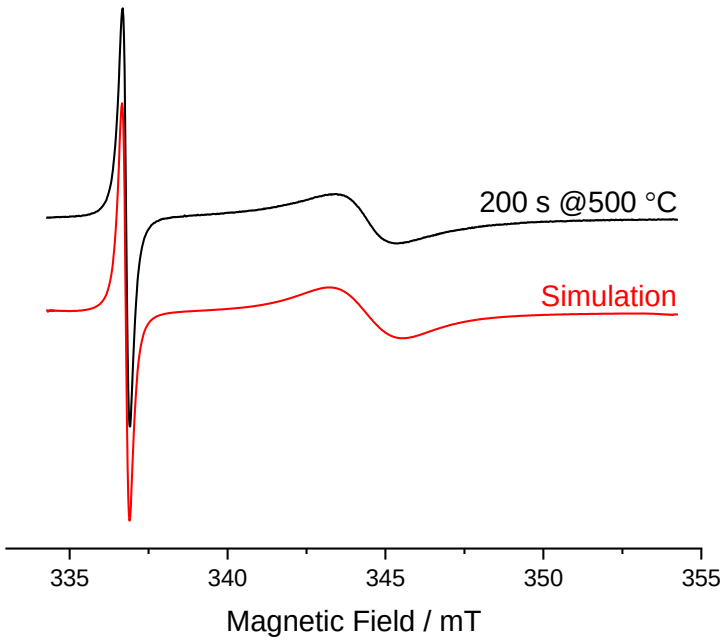

Figure S4. Simulation (red line) of the EPR spectrum of the ZHC sample annealed at 500 °C for 200 s (black line).

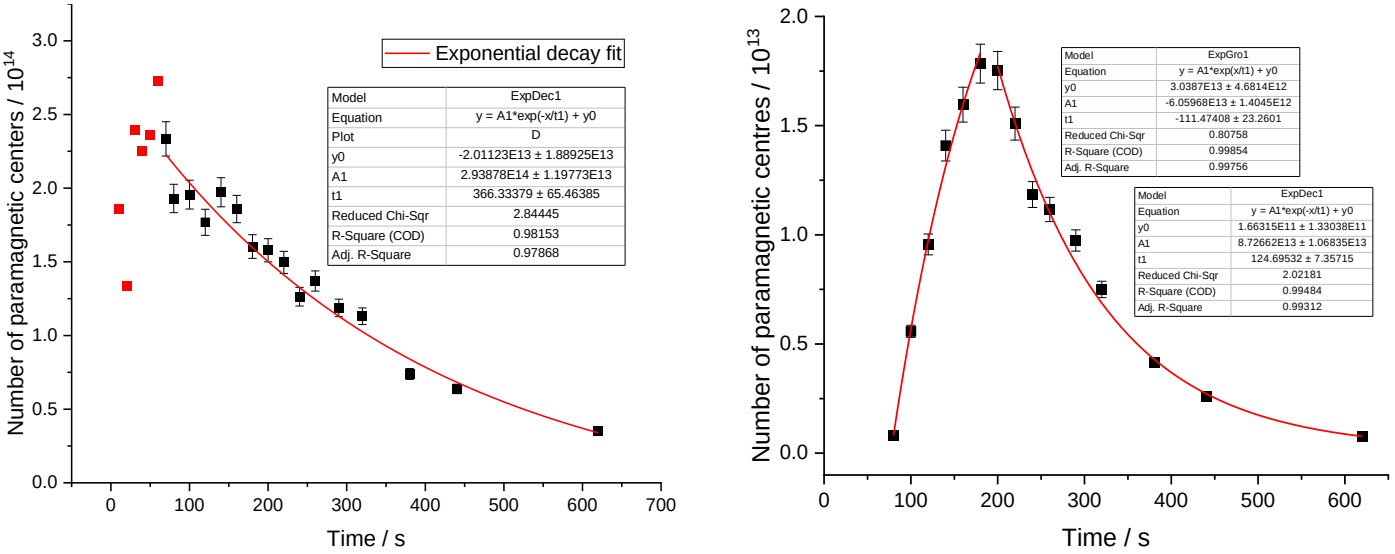

Figure S5. The reaction that characterizes the thermal decomposition of the ZHC nanoplatelets together with the SD signal decrease follow a mono-exponential decay function with a rate constant of k_{ZHC} = 0.16 ± 0.02 min^{-1} (left). The first six time points were not included in the fit, since it has to be taken into account that at the beginning of the thermal decomposition major structural changes take place, which lead to strong EPR signal fluctuations. The growth of the ZnO nanocrystals follows a more complex pattern. There are two main kinetic processes that take place in the thermal transformation of ZHC. In the first part of the kinetic t < 200 s the nanocrystals EPR signal starts growing, with a rate constant k_1 = 0.54±0.11 min^{-1} following a mono-exponential growth function (right). After an annealing time of 200 s the EPR signal decreases until it almost disappears with a rate constant k_2 =0.48±0.02 min^{-1} following a mono-exponential decay function. The fit parameters are summarized in the tables of each figure.