Supporting Information

Thermal decomposition of sodium amide, NaNH$_2$, and sodium amide hydroxide composites, NaNH$_2$–NaOH

Lars H. Jepsen$^a$, b Peikun Wang$^c$, Guotao Wu$^c$, Zhitao Xiong$^c$, Flemming Besenbacher$^d$, Ping Chen$^c$

and Torben R. Jensen$^a$

$^a$Center for Materials Crystallography, Interdisciplinary Nanoscience Center and Department of Chemistry, Aarhus University, Langelandsgade 140, DK-8000 Aarhus C, Denmark

$^b$Danish Technological Institute, Kongsvang Alle 29, 8000 Aarhus C, Denmark

$^c$Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023, P.R. China

$^d$Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, DK-8000 Aarhus C, Denmark.

*Corresponding author
Figure S1 Rietveld refinement of SR-PXD data for 0.33NaNH$_2$-0.67NaOH (s12) measured at 177 °C, $\lambda$ = 0.69449 Å. Tic marks NaOH, 31.8 wt% (top) and Na(OH)$_{1-x}$(NH$_2$)$_x$, 68.2 wt%. The following agreement factors were obtained for Na(OH)$_{1-x}$(NH$_2$)$_x$: $R_B$ = 4.95 %, $R_F$ = 6.63 %, $R_p$ = 1.73 %, $R_{wp}$ = 2.99 % (not corrected for background) and $\chi^2 = 0.204 \cdot 10^4$ (this value is high because of the very high counting statistics accumulated by the 2D detector).
Figure S2 In-situ SR-PXD of 0.33NaNH$_2$-0.67NaOH (s12) during heating from RT to 250 °C (5 °C/min, $\lambda$ = 0.69449 Å). The temperature difference between each PXD pattern is approx. 2 °C. A zoom of this data in the 2θ range 6.3° to 7.8° is shown in Figure 1a. Symbols: △ NaNH$_2$; □ NaOH; ▲Na(OH)$_{1-x}$(NH$_2$)$_x$. 
Figure S3 FTIR spectrum collected at RT for 0.70NaNH₂-0.30NaOH (s8) heated to 160 °C.
Figure S4 *In-situ* SR-PXD of NaNH$_2$ (s2) measured during heating from RT to 200 °C and subsequent cooling to RT (± 5 °C/min, $\lambda = 0.39997$ Å). Symbols: △ NaNH$_2$; □ NaOH; ▼ Na(OH)$_{1-x}$(NH$_2$)$_x$.
Figure S5 *In-situ* SR-PXD of 0.60NaNH$_2$-0.40NaOH (s10) measured during heating from RT to 175 °C and subsequent cooling to RT (± 5 °C/min, λ = 0.39997 Å). Symbols: △ NaNH$_2$; □ NaOH; ▼Na(OH)$_{1-x}$(NH$_2$)$_x$; ■ u1.
Figure S6 In-situ SR-PXD of 0.72NaNH$_2$-0.28NaOH (s7) measured during heating from RT to 175 °C and subsequent cooling to RT (± 5 °C/min, $\lambda = 0.39997$ Å). Symbols: △ NaNH$_2$; □ NaOH; ▼Na(OH)$_{1-x}$(NH$_2$)$_x$; ■ u1.
Figure S7 In-situ SR-PXD of 0.74NaNH$_2$-0.26NaOH (s6) measured during heating from RT to 165 °C and subsequent cooling to RT (± 5 °C/min, $\lambda = 0.39997$ Å). Symbols: Δ NaNH$_2$; □ NaOH; ▼Na(OH)$_{1-x}$(NH$_2$)$_x$; ■ u1.
Figure S8 In-situ SR-PXD of 0.77NaNH$_2$-0.23NaOH (s5) measured during heating from RT to 175 °C and subsequent cooling to 75 °C (± 3.5 °C/min, $\lambda = 0.9937$ Å). Symbols: $\Delta$ NaNH$_2$; $\Box$ NaOH; $\blacktriangle$ Na(OH)$_{1-x}$(NH$_2$)$_x$; $\blacksquare$ u1.
Figure S9 Temperature-programmed photographic analysis (TPPA) at 4 °C/min under argon atmosphere for xNaNH$_2$–(1-x)NaOH (x = 1 and 0.77, s2 and s5)

Figure S10 A picture of the glass tube after heating it with NaNH$_2$. 