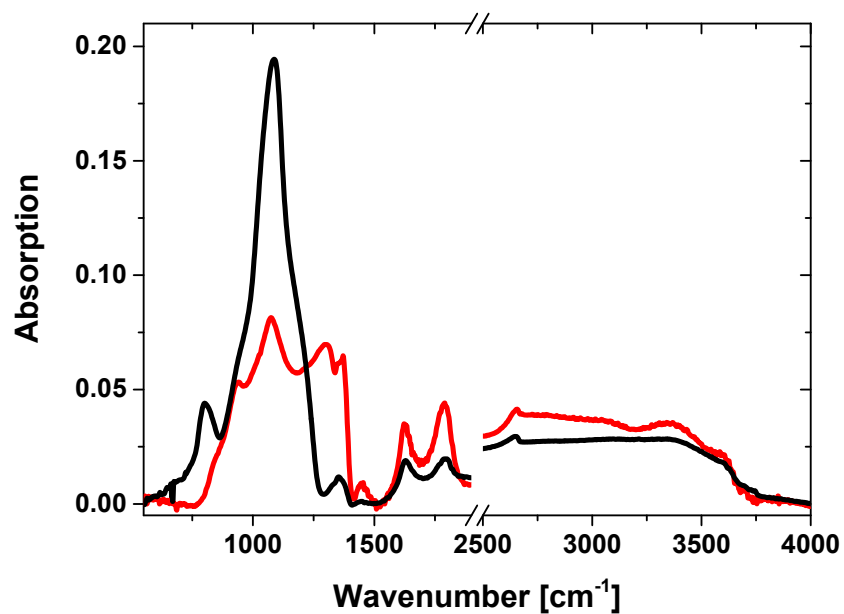


## Defined functionality and increased luminescence of nanodiamonds for sensoric and diagnostic applications by targeted high temperature reactions and electron beam irradiation

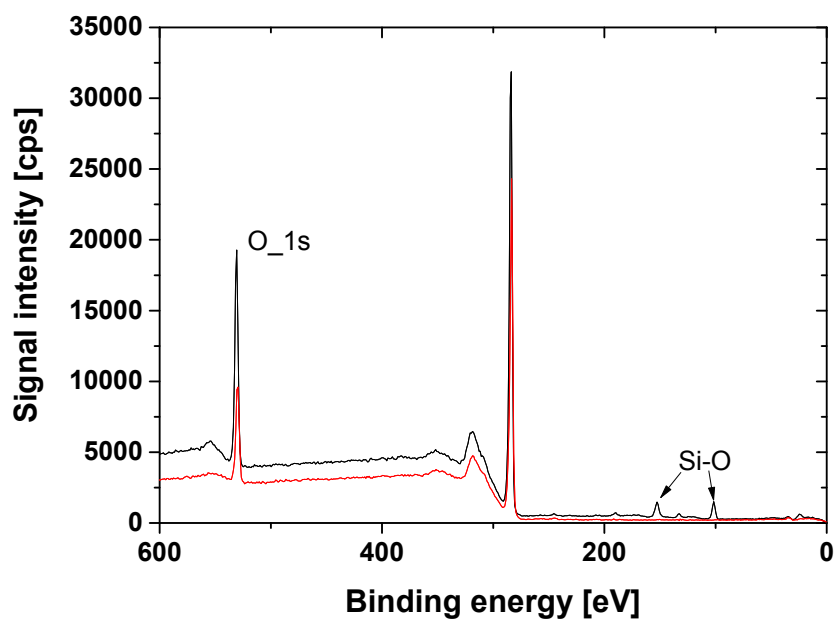
Ch. Laube,<sup>a,b</sup> Y. M. Riyad,<sup>a</sup> A. Lotnyk,<sup>a</sup> F.P. Lohmann,<sup>a</sup> C. Kranert,<sup>c</sup> R. Hermann,<sup>a</sup> W. Knolle,<sup>a</sup> Th.  
Oeckinghaus<sup>d</sup>, R. Reuter<sup>d</sup>, A. Denisenko,<sup>d</sup>, A. Kahnt,<sup>e</sup> and B. Abel<sup>a,b</sup>

### Supplementary information (SI)

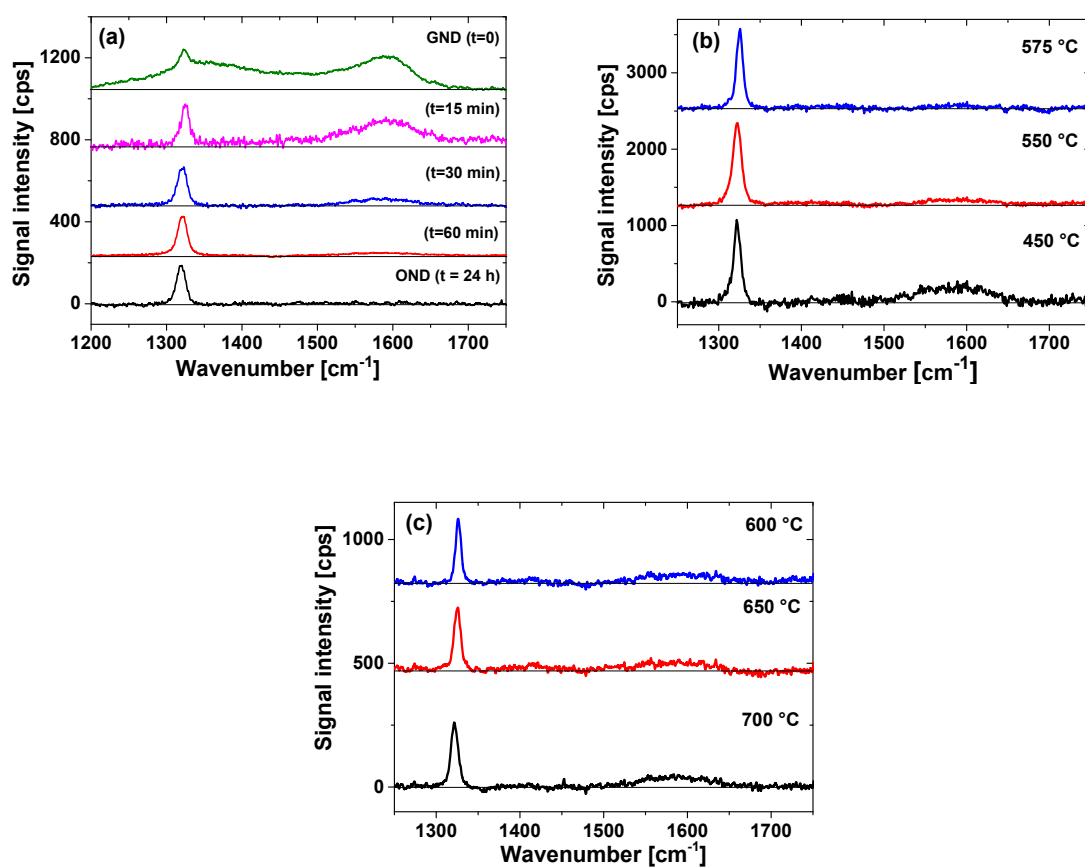
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- <sup>a.</sup> Leibniz-Institut für Oberflächenmodifizierung (IOM), Permoserstr. 15, D-04303 Leipzig, Germany  
<sup>b.</sup> *Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, University of Leipzig, Permoserstr. 15, 04318 Leipzig, Germany.*  
<sup>c.</sup> *Universität Leipzig, Institut für Experimentelle Physik II, Halbleiterphysik, Linnéstr. 5, 04103 Leipzig, Germany.*  
<sup>d.</sup> *3<sup>rd</sup> Institute of Physics, Research Center SCoPE and IQST, University of Stuttgart, 70569 Stuttgart, Germany*  
<sup>e.</sup> *Department of Chemistry and Pharmacy & Interdisciplinary Center for Molecular Materials, Chair of Physical Chemistry I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen, Germany.*



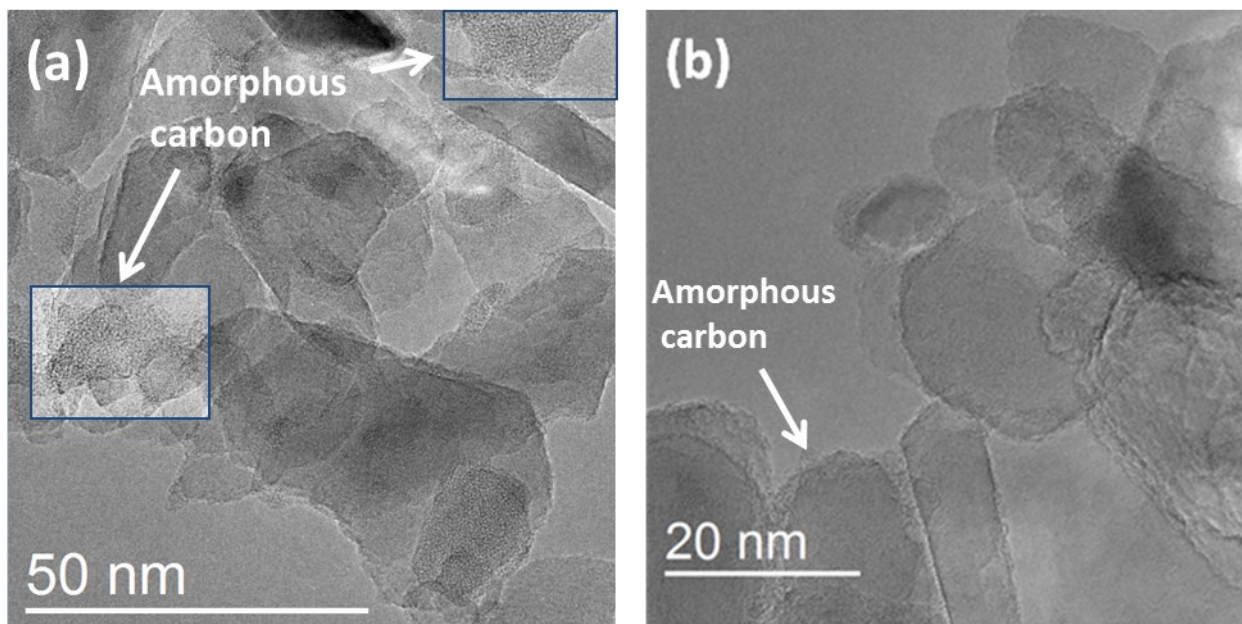
**Fig. S1** Removal of SiO<sub>2</sub> from the OND, ATR-IR spectra of: OND before HF/NH<sub>4</sub>F treatment (black) and after the treatment (red).



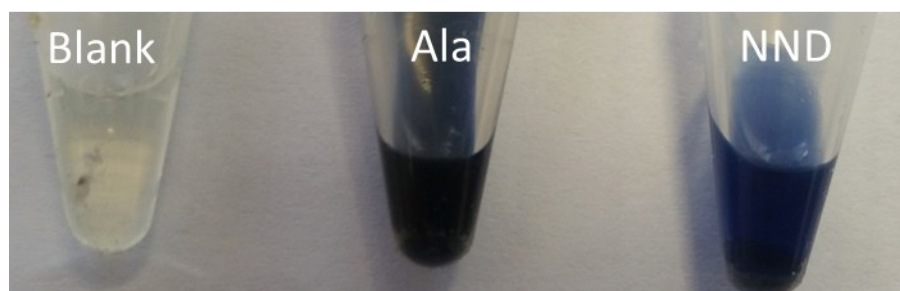
**Fig. S2** Removal of SiO<sub>2</sub> from the OND XPS spectra of: OND before HF/NH<sub>4</sub>F treatment (black), after treatment (red).



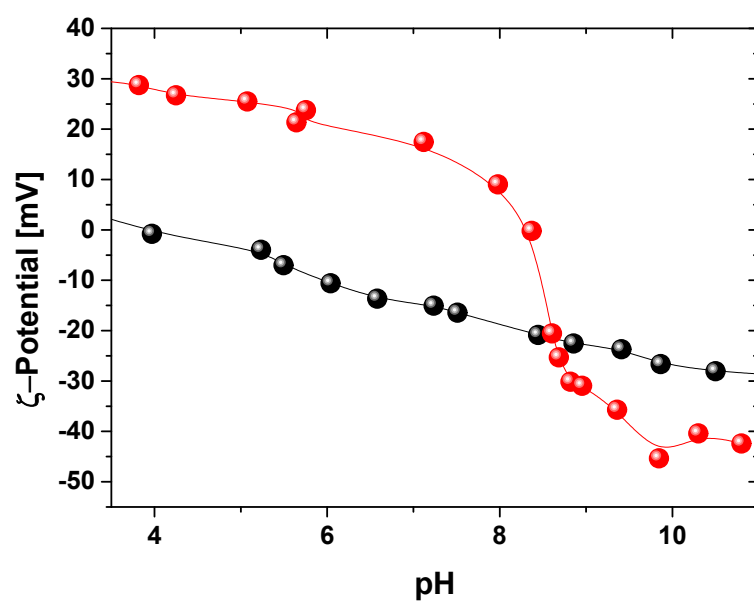
**Fig. S3** Raman spectra observation of degraphitisation and modification a) Duration time dependence for treatment of GND in air atmosphere at 590 °C; b) temperature dependence for treatment of GND in air atmosphere with a duration time of 24 hours; c) Nitrogen termination of OND in NH<sub>3</sub>- atmosphere at different temperatures with a duration time of 5 h.



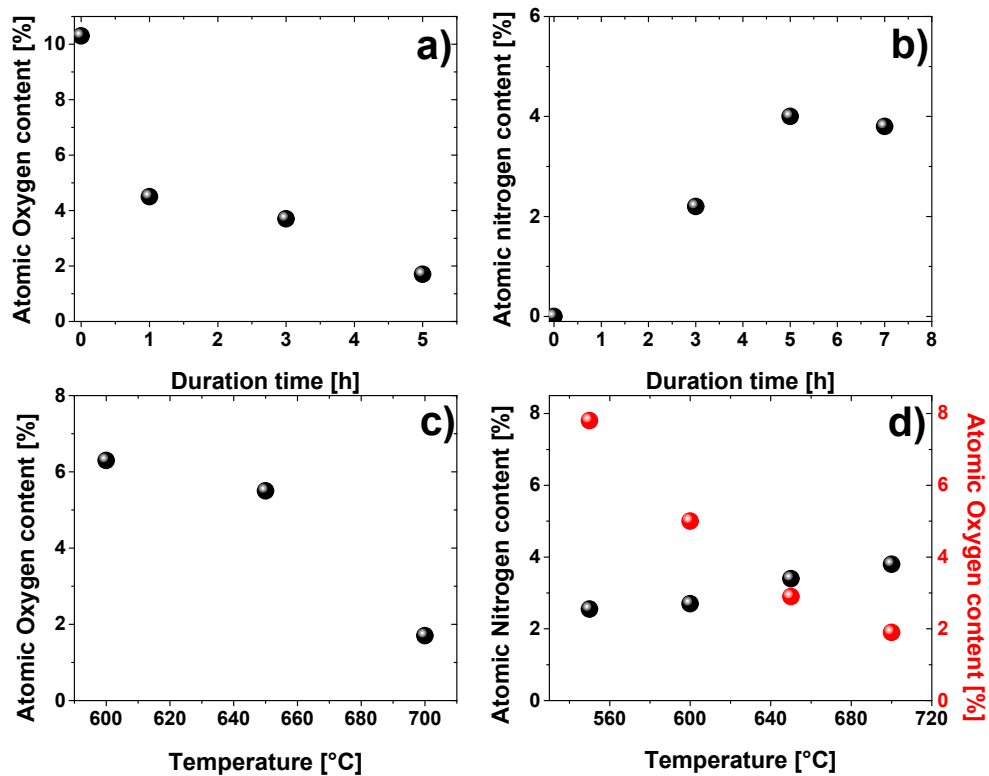
**Fig. S4** HRTEM image of NND samples a) prepared 700 °C ,7h; b) 600 °C 5 h).



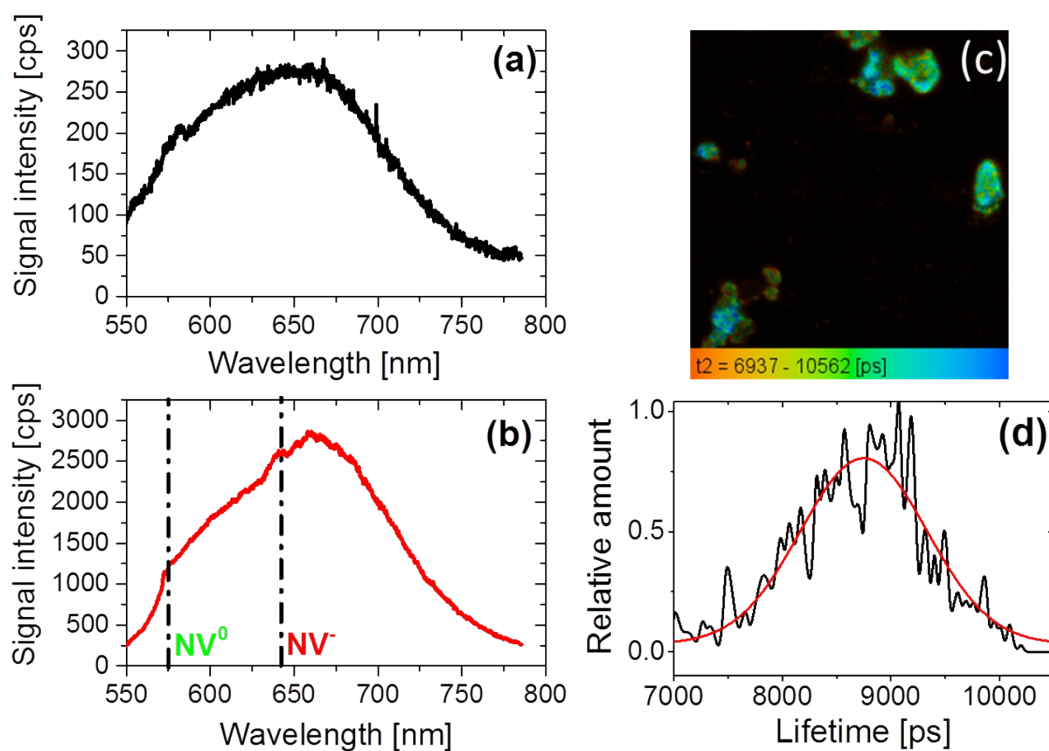
**Fig. S5** Representative results of a Kaisertest for NND prepared a 700 °C for 5 h: **left**: NND sample in water, **middle**: positive probe using alanine; **right**: positive result of NND.



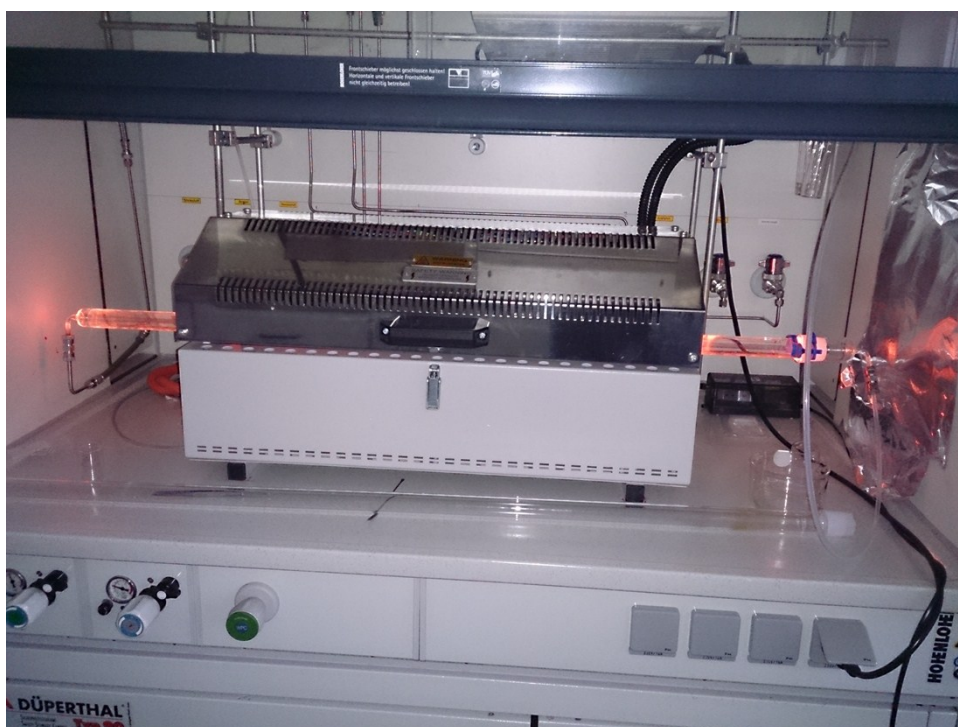
**Fig. S6** pH-value dependent measurements of the  $\zeta$ -potential of HND (black) and treated GND sample treated with hydrogen at 700 °C for 5 hours (red).



**Fig. S7** Process control of hydrogen and nitrogen termination starting from OND by XPS measurements a) atomic oxygen content of HND as a function of the duration in hydrogen atmosphere at 700 °C; b) atomic nitrogen content of NND as a function of the duration in ammonia atmosphere at 700 °C; c) Atomic oxygen content as a function of the reaction temperature in hydrogen atmosphere; d) atomic nitrogen and oxygen content of NND as a function of the reaction temperature in ammonia atmosphere.



**Fig. S8** Fluorescence properties of OND a) Fluorescence spectra of GND upon photoexcitation at 532 nm. The origin of the fluorescence is the non-diamond carbon; b) fluorescence spectra of OND upon excitation at 532 nm, the spectra shape is typical for  $NV^0$ -,  $NV^-$ -center with zero phonon lines at 575 nm and 639 nm; c) Fluorescence lifetime image ( $30\ \mu\text{m} \times 30\ \mu\text{m}$ ) of OND upon excitation at 513 nm; d) lifetime histogram determined from figure S7c.



**Fig. S9** Reactor for gas phase – solid phase reactor for hydrogen (C-H), oxygen and nitrogen termination (-NH<sub>2</sub>). Upper panel: open reactor; lower panel: reactor in operation with tight gas connections.