Supplementary materials to the article

Dedicated to 80-s birthday of academician K. Salikhov

Surface hydroxyl OH defects of η- Al_2O_3 and χ-Al_2O_3 by solid state NMR, XRD, and DFT calculations

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Figure S1. Experimental X-Ray diffraction patterns for χ-Al_2O_3: a - initial oxide, b - after annealing of the carbon coating. Vertical bars correspond to the spinel peaks.

Figure S2. Experimental X-Ray diffraction patterns for η-Al_2O_3: a - initial oxides, b - after annealing of the carbon coating. Vertical bars correspond to the spinel peaks.

Figure S3. ^{27}Al MAS NMR spectrum (15kHz) for χ-Al_2O_3 and η-Al_2O_3. Experimental spectrum of χ-Al_2O_3 with all spinning sidebands (a); central transition of χ-Al_2O_3 with its deconvolution (b); central transition of η-Al_2O_3 with its deconvolution (c).

Figure S4. ^{1}H MAS NMR spectra for χ-Al_2O_3 and η-Al_2O_3 : a – initial oxides, b – after H-D exchange, c – with carbon coating, d – after annealing of the carbon coating.

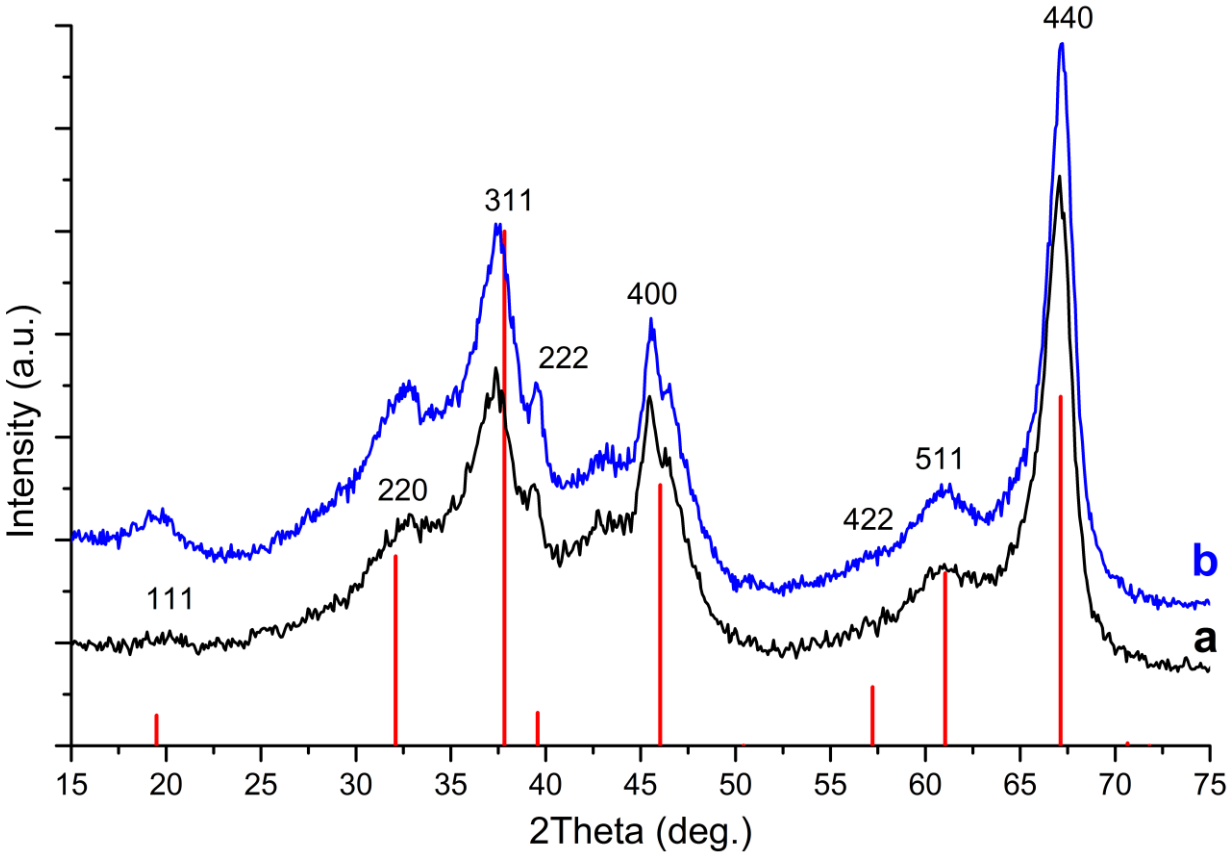
Figure S5. ^{1}H MAS NMR spectra of the initial χ-Al_2O_3 (a), after H-D exchange (b), and after annealing of the carbon coating (c) with deconvolution on individual lines

Figure S6. ^{1}H MAS NMR spectra of the initial η-Al_2O_3 (a), after H-D exchange (b), and after annealing of the carbon coating with deconvolution on individual lines

Figure S7. Theoretical ^{1}H MAS NMR spectra of the planes 100, 110, 111, 100-2, 110-2, 111-2

Figure S8. Theoretical ^{1}H -^{27}Al HETCOR NMR spectra for the planes 100, 110, 111, 100-2, 110-2, 111-2

Table S1 Structures of different planes



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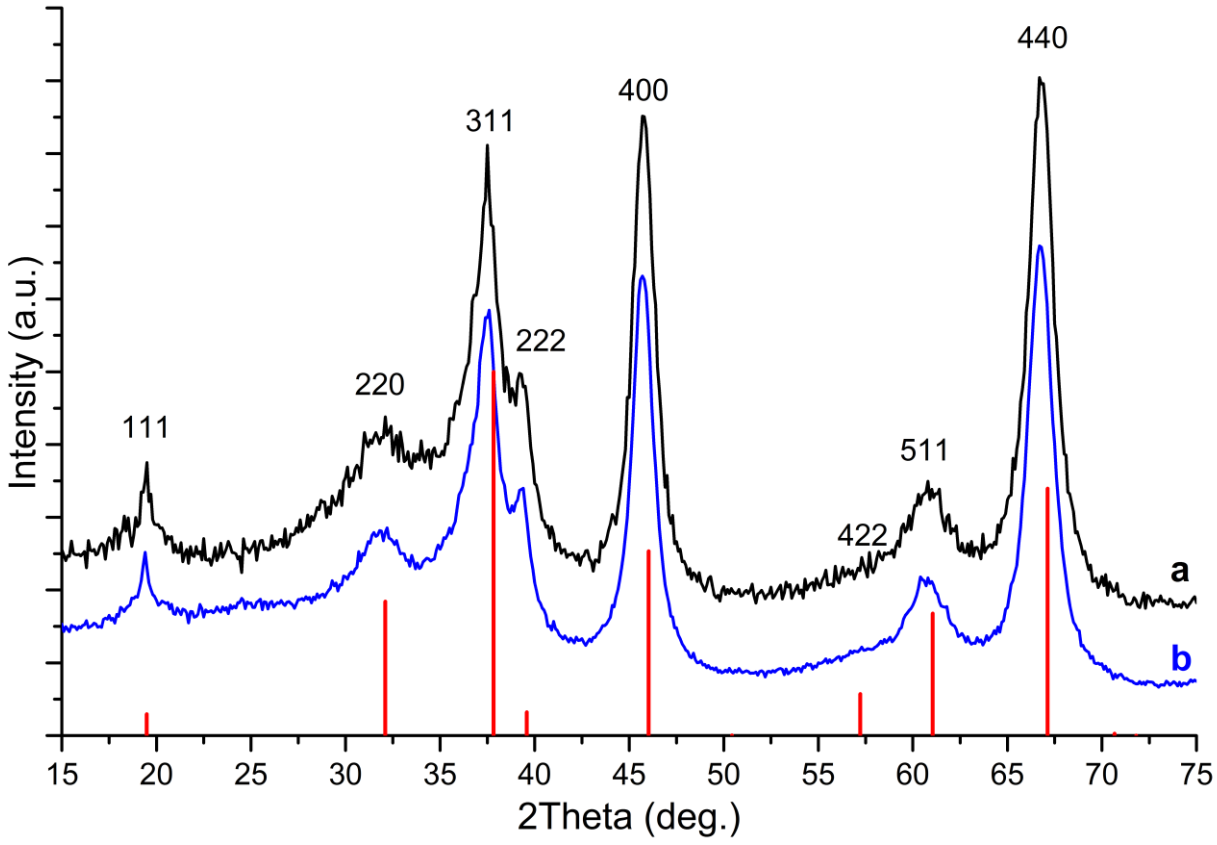
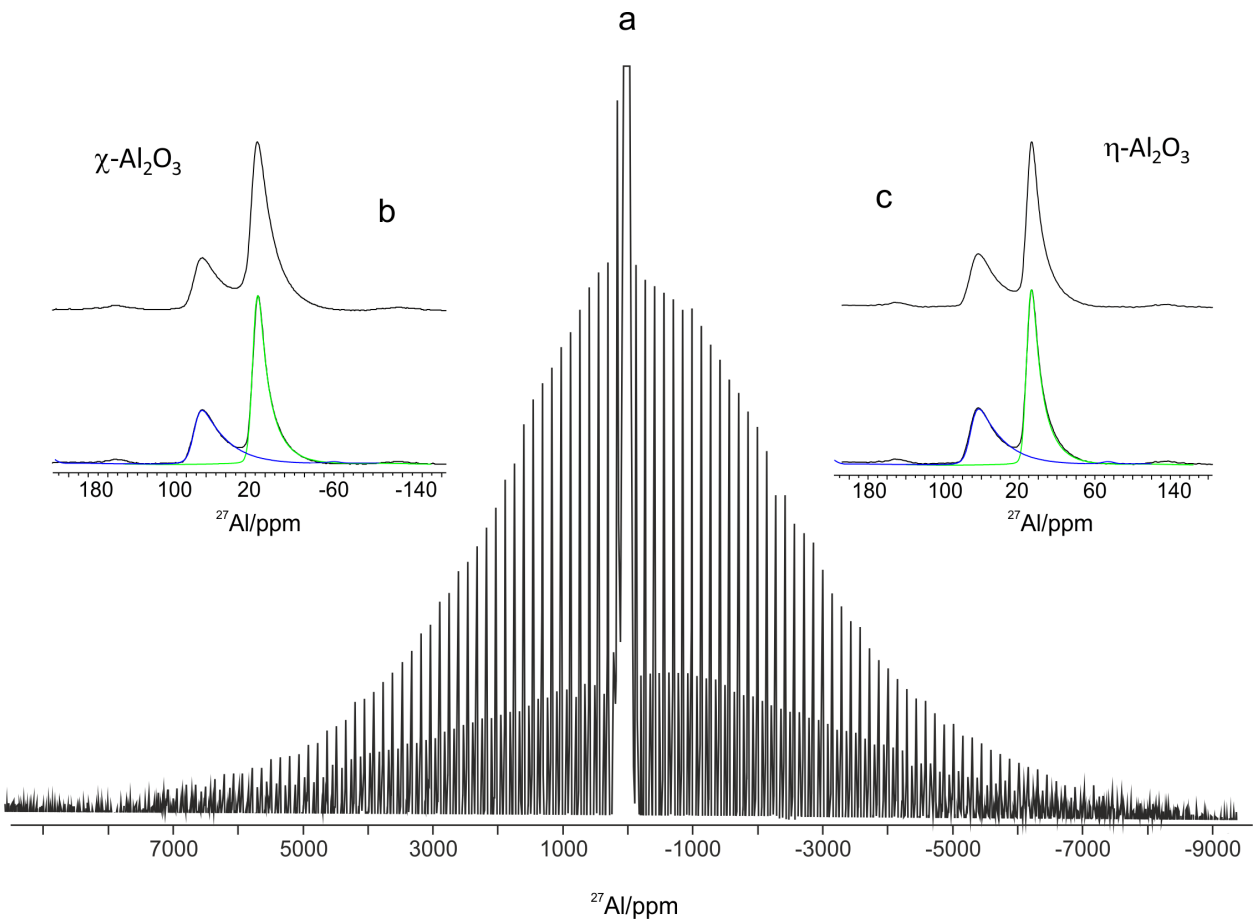


Figure S2. Experimental X-Ray diffraction patterns for η-Al_2O_3: a - initial oxides, b - after annealing of the carbon coating. Vertical bars correspond to the spinel peaks.



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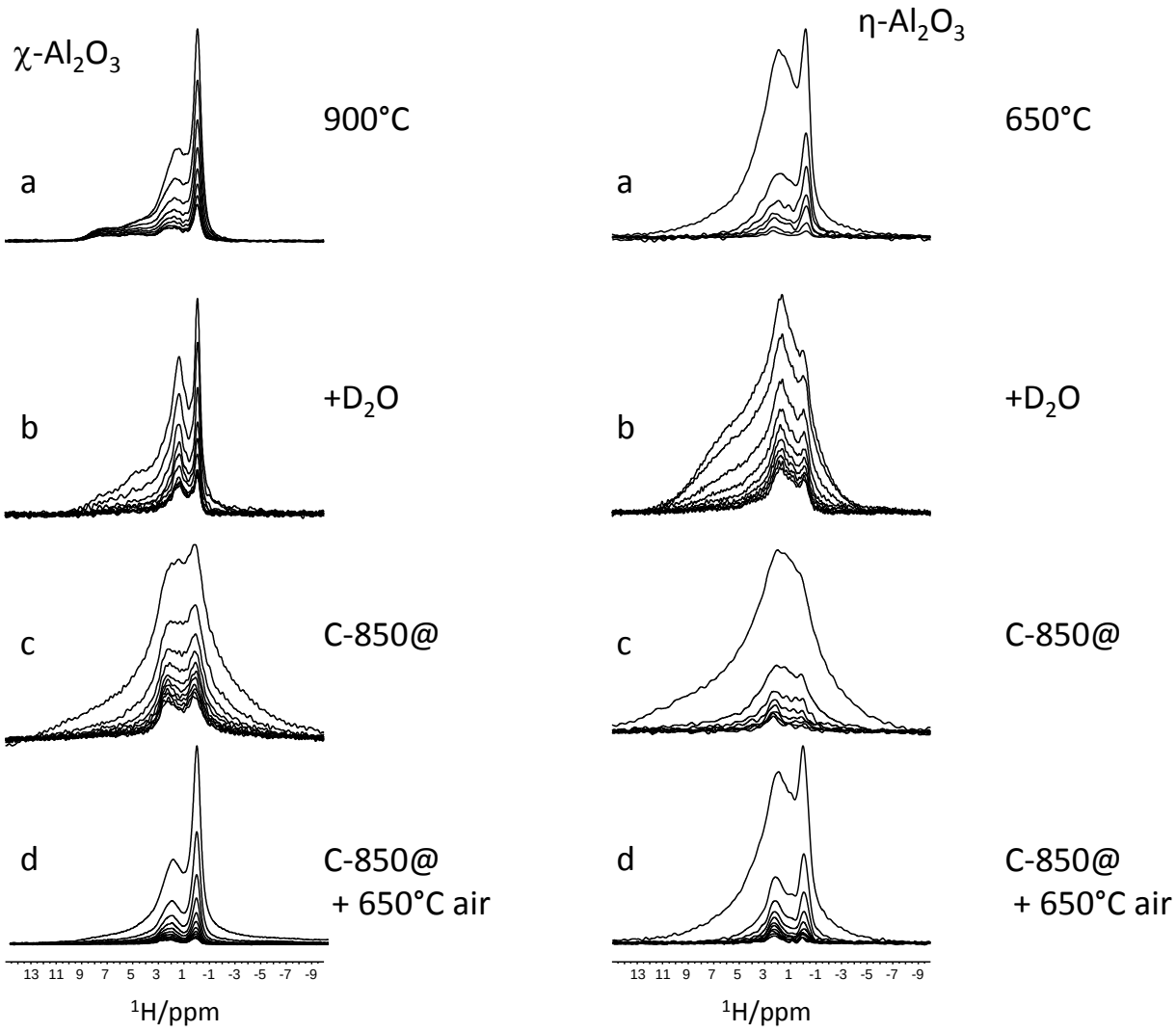
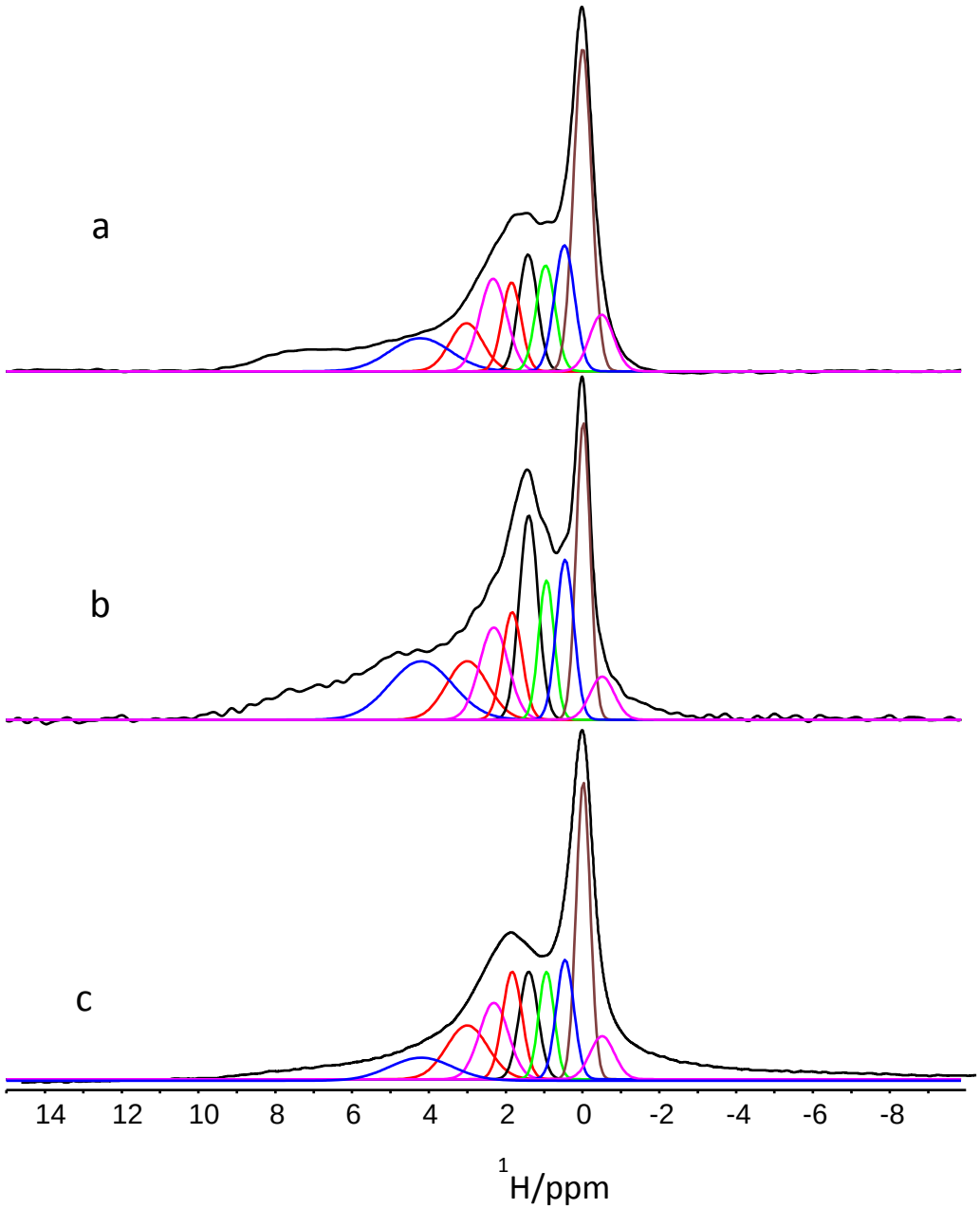


Figure S4. ^{1}H MAS NMR spectra for χ-Al_2O_3 and η-Al_2O_3 : a – initial oxides, b – after H-D exchange, c – with carbon coating, d – after annealing of the carbon coating.



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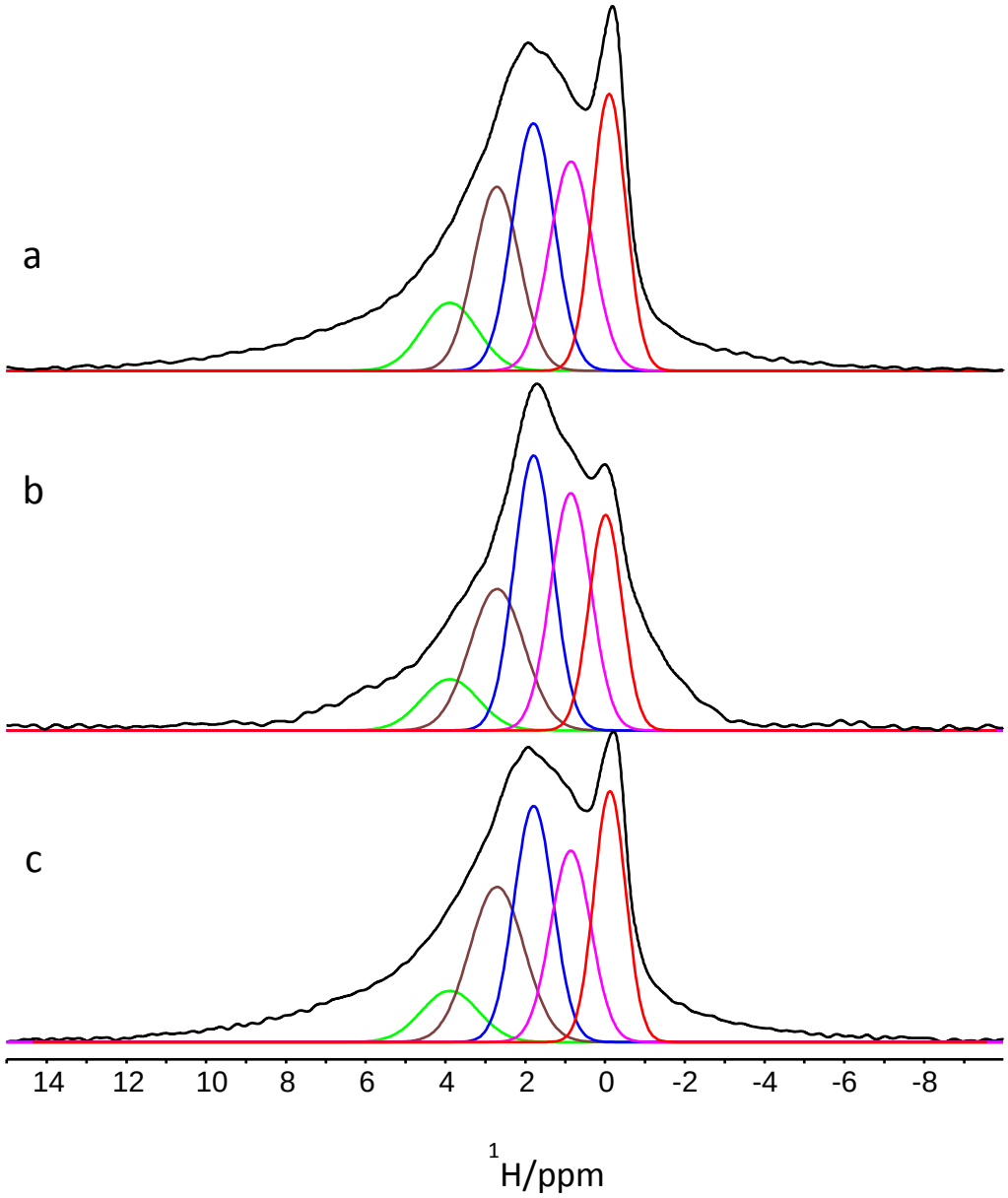
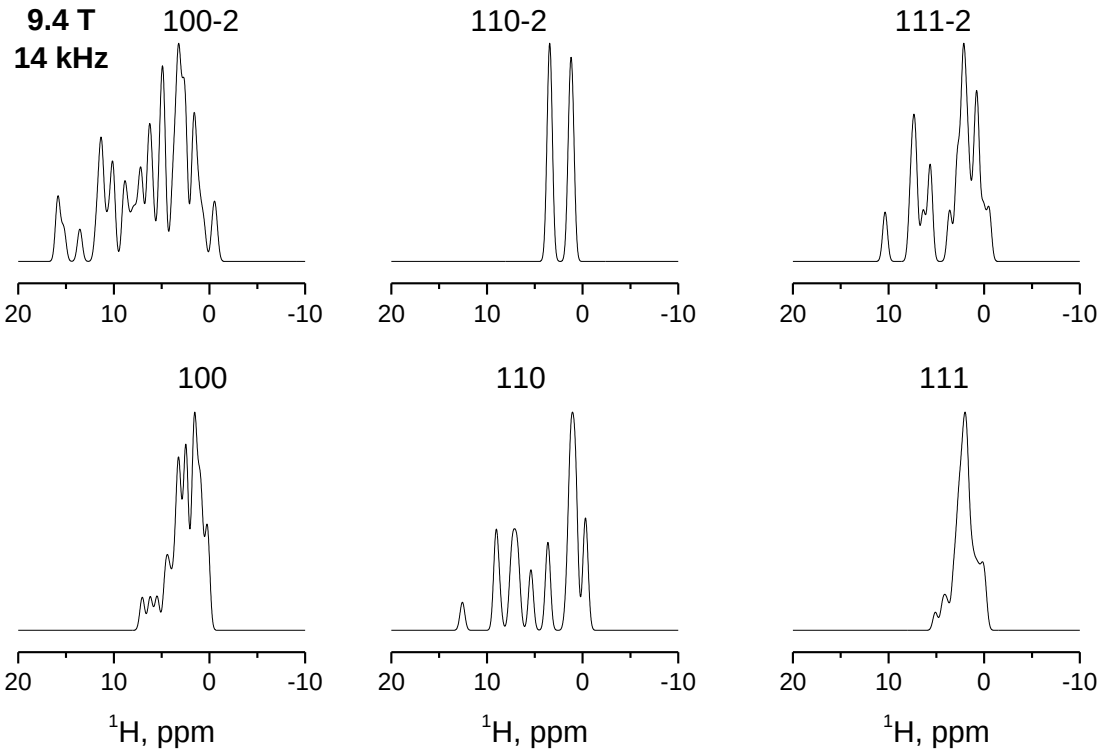


Figure S6. ^{1}H MAS NMR spectra of the initial η-Al_2O_3 (a), after H-D exchange (b), and after annealing of the carbon coating with deconvolution on individual lines.



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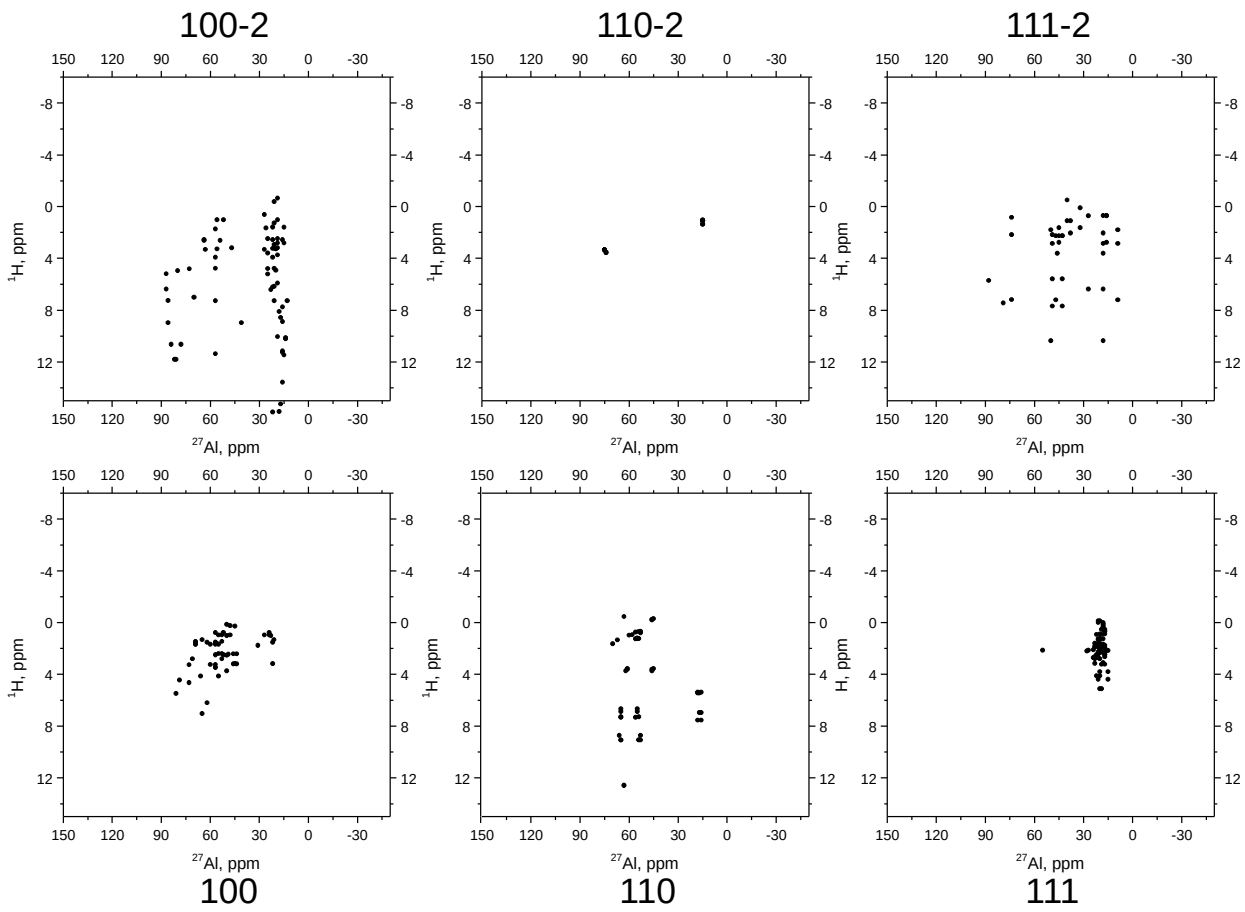

Figure S8. Theoretical ^{1}H -^{27}Al HETCOR NMR spectra for the planes 100, 110, 111, 100-2, 110-2, 111-2.

Table S1. Structures of different planes.

Structure	100	100-2	110	110-2	111	111-2
Number of H atoms	32	56	32	32	41	23
Surface density of H/S, $Å^{-2}$	0.122	0.214	0.087	0.087	0.181	0.102
OH group density, $Å^{-2}$	0.114	0.153	0.087	0.087	0.181	0.102