

**Andrew J Pell publication list**

---

51. A Bertarello, L Benda, KJ Sanders, **AJ Pell**, MJ Knight, V Pelmeshnikov, L Gonnelli, IC Felli, M Kaupp, L Emsley, R Pierattelli, G Pintacuda, Picometer resolution structure of the coordination sphere in the metal-binding site in a metalloprotein by NMR, *J Am Chem Soc*, **142**, 16757–16765 (2020). <https://doi.org/10.1021/jacs.0c07339>
50. M Winterlich, CG Efthymiou, W Papawassiliou, JP Carvalho, **AJ Pell**, J Mayans, A Escuer, MP Carty, P McArdle, E Tyllianakis, L Morrison, G Froudakis, C Papatriantafyllopoulou, A biocompatible ZnNa<sub>2</sub>-based metal-organic framework with high ibuprofen, nitric oxide and metal uptake capacity, *Mater Adv*, **1**, 2248–2260 (2020). <https://doi.org/10.1039/D0MA00450B> – *showcased article*
49. I Szewczyk, A Rokicińska, M Michalik, J Chen, A Jaworski, R Aleksis, **AJ Pell**, N Hedin, A Slabon, P Kuśtrowski, Electrochemical denitrification and oxidative dehydrogenation of ethylbenzene over N-doped mesoporous carbon: atomic level understanding of catalytic activity by <sup>15</sup>N NMR spectroscopy, *Chem Mater*, **32**, 7263–7273 (2020). <https://doi.org/10.1021/acs.chemmater.0c01666>
48. D Georgouvelas, B Jalvo, L Valencia, W Papawassiliou, **AJ Pell**, U Edlund, AP Mathew, Residual lignin and zwitterionic polymer grafts on cellulose nanocrystals for antifouling and antibacterial applications, *ACS Appl Polym Mater*, **2**, 3060–3071 (2020). <https://doi.org/10.1021/acsapm.0c00212> – *cover article*
47. C Eklöf-Österberg, L Mazzei, EJ Granhed, G Wahnström, R Nedumkandathil, U Häussermann, A Jaworski, **AJ Pell**, SF Parker, NH Jalarvo, L Börjesson, M Karlsson, The role of oxygen vacancies on the vibrational motions of hydride ions in the oxyhydride of barium titanate, *J Mater Chem A*, **8**, 6360–6371 (2020). <https://doi.org/10.1039/c9ta11912d>
46. W Papawassiliou, A Jaworski, **AJ Pell**, JH Jang, Y Kim, S-C Lee, HJ Kim, Y Alwahedi, S Alhassan, A Subrati, M Fardis, M Karagianni, N Panopoulos, J Dolinšek, G Papavassiliou, Resolving Dirac electrons with broadband high-resolution NMR, *Nat Commun*, **11**, 1285 (2020). <https://doi.org/10.1038/s41467-020-14838-4>
45. N Wahlström, U Edlund, H Pavia, G Toth, A Jaworski, **AJ Pell**, FX Choong, H Shirani, KPR Nilsson, A Richter-Dahlfors, Cellulose from the green macroalgae *Ulva lactuca*: isolation, characterization, optotracing, and production of cellulose nanofibrils, *Cellulose*, **27**, 3707–3725 (2020). <https://doi.org/10.1007/s10570-020-03029-5>
44. JP Carvalho, A Jaworski, MJ Brady, **AJ Pell**, Separation of quadrupolar and paramagnetic shift interactions with TOP-STMAS/MQMAS in solid-state lighting phosphors, *Magn Reson Chem*, **58**, 1055–1070 (2020). <https://doi.org/10.1002/mrc.5004> – *invited article for “Solid-State NMR for Materials Sciences” Special Issue*
43. Z Ma, A Jaworski, J George, A Rokicinska, T Thersleff, TM Budnyak, G Hautier, **AJ Pell**, R Dronskowski, P Kuśtrowski, A Slabon, Exploring the origins of improved photocurrent by acidic treatment for quaternary tantalum-based oxynitride photoanodes on the example of CaTaO<sub>2</sub>N, *J Phys Chem C*, **124**, 152–160 (2020). <https://doi.org/10.1021/acs.jpcc.9b09838>
42. D Eklöf, A Fischer, A Ektarawong, A Jaworski, **AJ Pell**, J Grins, SI Simak, B Alling, Y Wu, M Widom, W Scherer, U Häussermann, Mysterious SiB<sub>3</sub>: Identifying the relation between  $\alpha$ - and  $\beta$ -SiB<sub>3</sub>, *ACS Omega*, **4**, 18741–18759 (2019). <https://doi.org/10.1021/acsomega.9b02727>
41. WR Brant, R Mogensen, S Colbin, DO Ojwang, S Schmid, L Häggström, T Ericsson, A Jaworski, **AJ Pell**, R Younesi, Selective control of composition in Prussian white for enhanced material properties, *Chem Mater*, **31**, 7203–7211 (2019). <https://doi.org/10.1021/acs.chemmater.9b01494>
40. P Rzepka, Z Bacsik, **AJ Pell**, N Hedin, A Jaworski, Nature of chemisorbed CO<sub>2</sub> in zeolite A, *J Phys Chem C*, **123**, 21497–21503 (2019). <https://doi.org/10.1021/acs.jpcc.9b04142>
39. R Pigliapochi, L O’Brien, **AJ Pell**, MW Gaultois, Y Janssen, PG Khalifah, CP Grey, When do anisotropic magnetic susceptibilities lead to large NMR shifts? Exploring particle shape effects in the battery electrode material LiFePO<sub>4</sub>, *J Am Chem Soc*, **141**, 13089–13100 (2019). <https://doi.org/10.1021/jacs.9b04674>
38. AS Etman, **AJ Pell**, P Svedlindh, N Hedin, X Zou, J Sun, D Bernin, Insights into the exfoliation process of V<sub>2</sub>O<sub>5</sub>·*n*H<sub>2</sub>O nanosheet formation using real-time <sup>51</sup>V NMR, *ACS Omega*, **4**, 10899–10905 (2019). <https://doi.org/10.1021/acsomega.9b00727>
37. J Schlagnitweit, S Friebe Sandoz, A Jaworski, I Guzzetti, F Aussenac, RJ Carbajo, E Chiarparin, **AJ Pell**, K Petzold, Observing an antisense drug complex in intact human cells by in-cell NMR, *ChemBioChem*, **20**, 2474–2478 (2019). <https://doi.org/10.1002/cbic.201900297>

36. R Aleksis, JP Carvalho, A Jaworski, **AJ Pell**, Artefact-free broadband 2D NMR for separation of quadrupolar and paramagnetic shift interactions, *Solid State Nucl Magn Reson*, **101**, 51–62 (2019). <https://doi.org/10.1016/j.ssnmr.2019.05.001> – **invited article for “pNMR” Special Issue, cover article**
35. **AJ Pell**, G Pintacuda, CP Grey, Paramagnetic NMR in solution and the solid state, *Prog Nucl Magn Reson Spectrosc*, **111**, 1–271 (2019). <https://doi.org/10.1016/j.pnmrs.2018.05.001> – **in top 1% most cited in the field of chemistry**
34. C Eklöf-Österberg, R Nedumkandathil, U Häussermann, A Jaworski, **AJ Pell**, M Tyagi, NH Jalarvo, B Frick, A Faraone, M Karlsson, Dynamics of hydride ions in metal hydride-reduced BaTiO<sub>3</sub> samples investigated with quasielastic neutron scattering, *J Phys Chem C*, **123**, 2019–2030 (2019). <https://doi.org/10.1021/acs.jpcc.8b08451> – **cover article**
33. R Nedumkandathil, A Jaworski, J Grins, D Bernin, M Karlsson, C Eklöf-Österberg, A Neagu, C-W Tai, **AJ Pell**, U Häussermann, Hydride reduction of BaTiO<sub>3</sub> – Oxyhydride versus O vacancy formation, *ACS Omega*, **3**, 11426–11438 (2018). <https://doi.org/10.1021/acsomega.8b01368>
32. E Mitoudi-Vagourdi, W Papawassiliou, S Müllner, A Jaworski, **AJ Pell**, P Lemmens, RK Kremer, M Johnsson, Synthesis and physical properties of the oxofluoride Cu<sub>2</sub>(SeO<sub>3</sub>)F<sub>2</sub>, *Inorg Chem*, **57**, 4640–4648 (2018). <https://doi.org/10.1021/acs.inorgchem.8b00372>
31. K Jaudzems, A Bertarello, SR Chaudhari, A Pica, D Cala-De Paepe, E Barbet-Massin, **AJ Pell**, I Akopjana, S Kotelovica, D Gajan, O Ouari, K Tars, G Pintacuda, A Lesage, Dynamic nuclear polarization-enhanced biomolecular NMR spectroscopy at high magnetic field with fast magic-angle spinning, *Angew Chem Int Ed*, **57**, 7458–7462 (2018). <https://doi.org/10.1002/anie.201801016>
30. MA Tsiamtouri, PK Allan, **AJ Pell**, JM Stratford, G Kim, RN Kerber, PCMM Magusin, DA Jefferson, CP Grey, Exfoliation of layered Na-ion anode material Na<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> for enhanced capacity and cyclability, *Chem Mater*, **30**, 1505–1516 (2018). <https://doi.org/10.1021/acs.chemmater.7b03753>
29. KJ Sanders, **AJ Pell**, S Wegner, CP Grey, G Pintacuda, Broadband MAS NMR spectroscopy in the low-power limit, *Chem Phys Lett*, **697**, 29–37 (2018). <https://doi.org/10.1016/j.cplett.2018.01.028>
28. R Pigliapochi, ID Seymour, C Merlet, **AJ Pell**, DT Murphy, S Schmid, CP Grey, Structural characterization of the Li-ion battery cathode materials LiTi<sub>x</sub>Mn<sub>2-x</sub>O<sub>4</sub> (0.2 ≤ x ≤ 1.5): A combined experimental <sup>7</sup>Li NMR and first-principles study, *Chem Mater*, **30**, 817–829 (2018). <https://doi.org/10.1021/acs.chemmater.7b04314>
27. A Mondal, MW Gaultois, **AJ Pell**, M Iannuzzi, CP Grey, J Hutter, M Kaupp, Large-scale computation of NMR shifts for paramagnetic solids using CP2K, *J Chem Theory Comput*, **14**, 377–394 (2018). <https://doi.org/10.1021/acs.jctc.7b00991> – **cover article**
26. **AJ Pell**, KJ Sanders, S Wegner, G Pintacuda, CP Grey, Low-power broadband solid-state MAS NMR of <sup>14</sup>N, *J Chem Phys*, **146**, 194202 (2017). <https://doi.org/10.1063/1.4983220>
25. NC George, J Brgoch, **AJ Pell**, C Cozzan, A Jaffe, G Dantelle, A Llobet, G Pintacuda, R Seshadri, BF Chmelka, Correlating local compositions and structures with the macroscopic optical properties of Ce<sup>3+</sup>-doped CaSc<sub>2</sub>O<sub>4</sub>, an efficient green-emitting phosphor, *Chem Mater*, **29**, 3538–3546 (2017). <https://doi.org/10.1021/acs.chemmater.6b05394>
24. R Nedumkandathil, A Jaworski, A Fischer, C Österberg, Y- C Lin, M Karlsson, J Grins, **AJ Pell**, M Edén, U Häussermann, Investigation of the order–disorder rotator phase transition in KSiH<sub>3</sub> and RbSiH<sub>3</sub>, *J Phys Chem C*, **121**, 5241–5252 (2017). <https://doi.org/10.1021/acs.jpcc.6b12902>
23. R Pigliapochi, **AJ Pell**, ID Seymour, CP Grey, D Ceresoli, M Kaupp, DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids, *Phys Rev B*, **95**, 054412 (2017). <https://doi.org/10.1103/PhysRevB.95.054412>
22. J Lee, ID Seymour, **AJ Pell**, SE Dutton, CP Grey, A systematic study of <sup>25</sup>Mg NMR in paramagnetic transition metal oxides: applications to Mg-ion battery materials, *Phys Chem Chem Phys*, **19**, 613–625 (2017). <https://doi.org/10.1039/c6cp06338a>
21. V D’Anna, S Norsic, D Gajan, K Sanders, **AJ Pell**, A Lesage, V Monteil, C Copéret, G Pintacuda, P Sautet, Structural characterization of the EtOH–TiCl<sub>4</sub>–MgCl<sub>2</sub> Ziegler–Natta precatalyst, *J Phys Chem C*, **120**, 18075–18087 (2016). <https://doi.org/10.1021/acs.jpcc.6b05313>
20. ID Seymour, DS Middlemiss, DM Halat, NM Trease, **AJ Pell**, CP Grey, Characterizing oxygen local environments in paramagnetic battery materials via <sup>17</sup>O NMR and DFT calculations, *J Am Chem Soc*, **138**, 9405–9408 (2016). <https://doi.org/10.1021/jacs.6b05747>

19. AL Michan, G Divitini, **AJ Pell**, M Leskes, C Ducati, CP Grey, Solid electrolyte interphase growth and capacity loss in silicon electrodes, *J Am Chem Soc*, **138**, 7918–7931 (2016). <https://doi.org/10.1021/jacs.6b02882>
18. **AJ Pell**, G Pintacuda, Broadband solid-state MAS NMR of paramagnetic systems, *Prog Nucl Magn Reson Spectrosc*, **84–85**, 33–72 (2015). <https://doi.org/10.1016/j.pnmrs.2014.12.002>
17. E Barbet-Massin, **AJ Pell**, JS Retel, LB Andreas, K Jaudzems, WT Franks, AJ Nieuwkoop, M Hiller, VA Higman, P Guerry, A Bertarello, MJ Knight, M Felletti, T Le Marchand, S Kotelovica, I Akopjana, K Tars, M Stoppini, V Bellotti, M Bolognesi, S Ricagno, JJ Chou, RG Griffin, H Oschkinat, A Lesage, L Emsley, T Herrmann, G Pintacuda, Rapid proton-detected NMR assignment for proteins with fast magic angle spinning, *J Am Chem Soc*, **136**, 12489–12497 (2014). <https://doi.org/10.1021/ja507382j> – *in top 1% most cited in the field of chemistry*
16. C Ferrara, C Tealdi, P Mustarelli, M Hoelzel, **AJ Pell**, G Pintacuda, The melilite  $\text{LaSrGa}_{3-x}\text{Al}_x\text{O}_7$  series: a combined solid-state NMR and neutron diffraction study, *J Phys Chem C*, **118**, 15036–15043 (2014). <https://doi.org/10.1021/jp504829x>
15. FC Strobridge, DS Middlemiss, **AJ Pell**, M Leskes, RJ Clément, F Pourpoint, Z Lu, JV Hanna, G Pintacuda, L Emsley, A Samoson, CP Grey, Characterising local environments in high energy density Li-ion battery cathodes: a combined NMR and first principles study of  $\text{LiFe}_x\text{Co}_{1-x}\text{PO}_4$ , *J Mater Chem A*, **2**, 11948–11957 (2014). <https://doi.org/10.1039/c4ta00934g>
14. J Xu, DH Lee, RJ Clément, X Yu, M Leskes, **AJ Pell**, G Pintacuda, X-Q Yang, CP Grey, YS Meng, Identifying the critical role of Li substitution in  $\text{P2-Na}_x[\text{Li}_y\text{Ni}_z\text{Mn}_{1-y-z}]\text{O}_2$  ( $0 < x, y, z < 1$ ) intercalation cathode materials for high-energy Na-ion batteries, *Chem Mater*, **26**, 1260–1269 (2014). <https://doi.org/10.1021/cm403855t> – *in top 1% most cited in the field of materials science*
13. M Bini, S Ferrari, C Ferrara, MC Mozzati, D Capsoni, **AJ Pell**, G Pintacuda, P Canton, P Mustarelli, Polymorphism and magnetic properties of  $\text{Li}_2\text{MSiO}_4$  (M = Fe, Mn) cathode materials, *Sci Rep*, **3**, 3452 (2013). <https://doi.org/10.1038/srep03452>
12. NC George, **AJ Pell**, G Dantelle, K Page, A Llobet, M Balasubramanian, G Pintacuda, BF Chmelka, R Seshadri, Local environments of dilute activator ions in the solid-state lighting phosphor  $\text{Y}_3\text{Al}_5\text{O}_{12}$ , *Chem Mater*, **25**, 3979–3995 (2013). <https://doi.org/10.1021/cm401598n>
11. E Barbet-Massin, **AJ Pell**, MJ Knight, AL Webber, IC Felli, R Pierattelli, L Emsley, A Lesage, G Pintacuda,  $^{13}\text{C}$ -detected through-bond correlation experiments for protein resonance assignment by ultra-fast MAS solid-state NMR spectroscopy, *ChemPhysChem*, **14**, 3131–3137 (2013). <https://doi.org/10.1002/cphc.201201097> – *invited article*
10. E Barbet-Massin, **AJ Pell**, K Jaudzems, WT Franks, JS Retel, S Kotelovica, I Akopjana, K Tars, L Emsley, H Oschkinat, A Lesage, G Pintacuda, Out-and-back  $^{13}\text{C}$ – $^{13}\text{C}$  scalar transfers in protein resonance assignment by proton-detected solid-state NMR under ultra-fast MAS, *J Biomol NMR*, **56**, 379–386 (2013). <https://doi.org/10.1007/s10858-013-9757-3>
9. **AJ Pell**, RJ Clément, CP Grey, L Emsley, G Pintacuda, Frequency-stepped acquisition in nuclear magnetic resonance spectroscopy under magic angle spinning, *J Chem Phys*, **138**, 114201 (2013). <https://doi.org/10.1063/1.4795001>
8. RJ Clément, **AJ Pell**, DS Middlemiss, FC Strobridge, JK Miller, MS Whittingham, L Emsley, CP Grey, G Pintacuda, Spin-transfer pathways in paramagnetic lithium transition metal phosphates from combined broadband isotropic solid-state MAS NMR spectroscopy and DFT calculations, *J Am Chem Soc*, **134**, 17178–17185 (2012). <https://doi.org/10.1021/ja306876u> – *spotlight article*
7. MJ Knight, **AJ Pell**, I Bertini, IC Felli, L Gonnelli, R Pierattelli, T Herrmann, L Emsley, G Pintacuda, Structure and backbone dynamics of a microcrystalline metalloprotein by solid-state NMR, *Proc Natl Acad Sci USA*, **109**, 11095–11100 (2012). <https://doi.org/10.1073/pnas.1204515109>
6. AL Webber, **AJ Pell**, E Barbet-Massin, MJ Knight, I Bertini, IC Felli, R Pierattelli, L Emsley, A Lesage, G Pintacuda, Combination of DQ and ZQ coherences for sensitive through-bond NMR correlation experiments in biosolids under ultra-fast MAS, *ChemPhysChem*, **13**, 2405–2411 (2012). <https://doi.org/10.1002/cphc.201200099>
5. MJ Knight, AL Webber, **AJ Pell**, P Guerry, E Barbet-Massin, I Bertini, IC Felli, L Gonnelli, R Pierattelli, L Emsley, A Lesage, T Herrmann, G Pintacuda, Fast resonance assignment and fold determination of the 153-residue protein superoxide dismutase by high-resolution proton-detected solid-state MAS NMR spectroscopy, *Angew Chem Int Ed*, **50**, 11697–11701 (2011). <https://doi.org/10.1002/anie.201106340>
4. **AJ Pell**, G Pintacuda, L Emsley, Single crystal nuclear magnetic resonance in spinning powders, *J Chem Phys*, **135**, 144201 (2011). <https://doi.org/10.1063/1.3640418> – *cover article*

3. **AJ Pell**, G Kervern, L Emsley, M Deschamps, D Massiot, PJ Grandinetti, G Pintacuda, Broadband inversion for MAS NMR with single-sideband-selective adiabatic pulses, *J Chem Phys*, **134**, 024117 (2011). <https://doi.org/10.1063/1.3521491>
2. **AJ Pell**, J Keeler, Two-dimensional *J*-spectra with absorption-mode lineshapes, *J Magn Reson*, **189**, 293–299 (2007). <https://doi.org/10.1016/j.jmr.2007.09.002>
1. **AJ Pell**, RAE Edden, J Keeler, Broadband proton-decoupled proton spectra, *Magn Reson Chem*, **45**, 296–316 (2007). <https://doi.org/10.1002/mrc.1966>