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13. **Juha Vaara** and Yrjö Hiltunen: *Deuterium quadrupole coupling tensors in methyl halides: Ab initio effective core potential and liquid crystal nuclear magnetic resonance study*, Journal of Chemical Physics **107**, 1744–1752 (1997).
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118. Jouni Karjalainen, **Juha Vaara**, Michal Straka and Perttu Lantto: *Xenon NMR of liquid crystals confined to cylindrical nanocavities: A simulation study*, *Physical Chemistry Chemical Physics* **17**, 7158 (2015).

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121. Jarkko Vähäkangas, Perttu Lantto, Jiří Mareš, and **Juha Vaara**: *Spin Doublet Point Defects in Graphenes: Predictions for ESR and NMR Spectral Parameters*, *Journal of Chemical Theory and Computation* **11**, 3746 (2015).
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123. Jyrki Rantaharju and **Juha Vaara**: *Liquid-state paramagnetic relaxation from first principles*, *Physical Review A* **94**, 043413:1–10 (2016).
124. Juho Roukala, Simon Orr, John V. Hanna, **Juha Vaara**, Alexander V. Ivanov, Oleg N. Antzutkin, and Perttu Lantto: *Experimental and first-principles NMR analysis of Pt(II) complexes with O,O-dialkylthiophosphate ligands*, *Journal of Physical Chemistry A* **120**, 8326–8338 (2016).
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126. Matti Hanni, Perttu Lantto, Michal Repiský, Jiří Mareš, Brian Saam, and **Juha Vaara**: *Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization*, *Physical Review A* **95**, 032509:1–10 (2017).
127. Peter John Cherry, Syed Awais Rouf, and **Juha Vaara**: *Paramagnetic enhancement of nuclear spin-spin coupling*, *Journal of Chemical Theory and Computation* **13**, 1275–1283 (2017).
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130. Jukka Jokisaari, Anu M. Kantola, and **Juha Vaara**: *Magnetic field-induced effects on NMR properties*, *Journal of Magnetic Resonance* **281**, 1–6 (2017).
131. Syed Awais Rouf, Vibe Boel Jakobsen, Jiří Mareš, Nicholai Daugaard Jensen, Christine McKenzie, **Juha Vaara**, and Ulla Gro Nielsen: *Assignment of solid-state  $^{13}\text{C}$  and  $^1\text{H}$  NMR spectra of paramagnetic Ni(II) acetylacetonate complexes aided by first-principles computations*, *Solid State Nuclear Magnetic Resonance* **87**, 29–37 (2017).
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133. Juho Roukala, Michal Straka, Stefan Taubert, **Juha Vaara**, and Perttu Lantto: *Ratcheting Rotation or Speedy Spinning: EPR and Dynamics of Sc<sub>3</sub>C<sub>2</sub>@C<sub>80</sub>*, *Chemical Communications* **53**, 8992–8995 (2017).
134. Bing Zhou, Sanna Komulainen, **Juha Vaara**, and Ville-Veikko Telkki: *Characterization of pore structures of hydrated cements and natural shales by  $^{129}\text{Xe}$  NMR spectroscopy*, *Microporous and Mesoporous Materials* **253**, 49–54 (2017).
135. Pär Håkansson, Tom Boirin, and **Juha Vaara**: *Brownian translational dynamics on a flexible surface: Nuclear spin relaxation of fluid membrane phases*, *Langmuir* **34**, 3755–3766 (2018).



136. Petri Peuravaara, Jouni Karjalainen, Jianfeng Zhu, Jiří Mareš, Perttu Lantto, and **Juha Vaara**: *Chemical shift extremum of  $^{129}\text{Xe}(\text{aq})$  reveals details of hydrophobic solvation*, *Scientific Reports* **8**, 7023 (2018).
137. Jiří Mareš and **Juha Vaara**: *Ab initio paramagnetic NMR shifts via point-dipole approximation in a large magnetic-anisotropy Co(II) complex*, *Physical Chemistry Chemical Physics* **20**, 22547–22555 (2018).
138. Jyrki Rantaharju, Matti Hanni, and **Juha Vaara**: *Polarization transfer in a spin-exchange optical-pumping experiment*, *Physical Review A* **102**, 032813:1–8 (2020).
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140. **Juha Vaara** and Michael V. Romalis: *Calculation of scalar nuclear spin-spin coupling in a noble gas mixture*, *Physical Review A (Rapid Communications)* **99**, 060501:1–5 (2019).
141. M. E. Limes, N. Dural, M. V. Romalis, E. L. Foley, T. W. Kornack, A. Nelson, L. R. Grisham, and **J. Vaara**: *Dipolar and scalar  $^3\text{He}$ - $^{129}\text{Xe}$  frequency shifts in stemless cells*, *Physical Review A (Rapid Communications)* **100**, 010501 (2019).
142. Anders B. A. Andersen, Ari Pyykkönen, Hans Jørgen Aagaard Jensen, Vickie McKee, **Juha Vaara**, and Ulla Gro Nielsen: *Remarkable reversal of  $^{13}\text{C}$ -NMR assignment in  $d^1$ ,  $d^2$  compared to  $d^8$ ,  $d^9$  acetylacetonate complexes: Analysis and explanation based on solid-state MAS NMR and computations*, *Physical Chemistry Chemical Physics* **22**, 8048–8059 (2020).
143. Anu M. Kantola, Perttu Lantto, Ivo Heinmaa, **Juha Vaara** and Jukka Jokisaari: *Direct magnetic-field dependence of NMR chemical shift*, *Physical Chemistry Chemical Physics* **22**, 8485–8490 (2020).
144. Ari Pyykkönen, Robert Feher, Frank H. Köhler, and **Juha Vaara**: *Paramagnetic Pyrazolylborate Complexes,  $\text{Tp}_2\text{M}$  and  $\text{Tp}_2^*\text{M}$ .  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{11}\text{B}$ , and  $^{14}\text{N}$  NMR Spectra and First-Principles Studies of Chemical Shifts*, *Inorganic Chemistry* **59**, 9294–9307 (2020).
145. Piotr Garbacz and **Juha Vaara**: *Direct enantiomeric discrimination through antisymmetric hyperfine coupling*, *Chemical Communications* **57**, 8264–8267 (2021).
146. Perttu Hilla and **Juha Vaara**: *Energetics and Exchange of Xenon and Water in a Prototypic Cryptophane-A Biosensor Structure*, *Physical Chemistry Chemical Physics* **24**, 17946–17950 (2022).
147. Ben Tickner, S. Karl-Mikael Svensson, **Juha Vaara**, and Simon Duckett: *Towards Optimising and Understanding Reversible Hyperpolarisation of Lactate Esters Relayed from Parahydrogen*, *Journal of Physical Chemistry Letters* **13**, 6859–6866 (2022).
148. Roya Khalili, Anu Kantola, Sanna Komulainen, Anne Selent, Marcin Selent, **Juha Vaara**, Anna-Carin Larsson, Perttu Lantto, and Ville-Veikko Telkki:  *$^{129}\text{Xe}$  NMR analysis of pore structures and adsorption phenomena in rare-earth element phosphates*, *Microporous and Mesoporous Materials* **344**, 112209 (2022).
149. Ari Pyykkönen and **Juha Vaara**: *Computational NMR of the iron pyrazolylborate complexes  $[\text{Tp}_2\text{Fe}]^+$  and  $\text{Tp}_2\text{Fe}$  including solvation and spin-crossover effects*, *Physical Chemistry Chemical Physics* **25**, 3121–3135 (2023).
150. Anders B. A. Andersen, Rasmus T. Christiansen, Sofie Holm-Janass, Anna Manvell, Kasper S. Pedersen, Denis Sheptyakov, Jan Embs, Henrik Jacobsen, Edgar Dachs, **Juha Vaara**, Kim Lefmann, and Ulla G. Nielsen: *The Magnetic Properties of  $\text{MAl}_4(\text{OH})_{12}\text{SO}_4 \cdot 3\text{H}_2\text{O}$   $\text{M} = \text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ , and  $\text{Cu}^{2+}$  Determined by a Combined Experimental and Computational Approach*, *Physical Chemistry Chemical Physics* **25**, 3309–3322 (2023).
151. Jan Vícha, **Juha Vaara** and Michal Straka: *The Essential Role of Symmetry in Understanding  $^3\text{He}$  Chemical Shifts in Endohedral Helium Fullerenes*, *Physical Chemistry Chemical Physics* **25**, 10620–10627 (2023).

152. **Juha Vaara**: *Quantum-Chemical Approach to Nuclear Magnetic Resonance of Paramagnetic Systems*, *Annales Academiae Scientiarum Fennicae* **2**, 96–115 (2023).
153. Perttu Hilla and **Juha Vaara**: *NMR chemical shift of confined Xe: Coordination number, paramagnetic channels and molecular dynamics in a cryptophane-A biosensor*, *Physical Chemistry Chemical Physics* **25**, 22719–22733 (2023).
154. Megha Mohan, Anders B. A. Andersen, Jiří Mareš, Nicholai Daugaard Jensen, Ulla Gro Nielsen and **Juha Vaara**: *Unravelling the effect of paramagnetic Ni<sup>2+</sup> on the <sup>13</sup>C NMR shift tensor for carbonate in Mg<sub>2-x</sub>Ni<sub>x</sub>Al layered double hydroxides by quantum-chemical computations*, *Physical Chemistry Chemical Physics* **25**, 24081–24096 (2023).
155. Eelis Kamula, **Juha Vaara**, and Petr Štěpánek: *Characteristic nuclear spin-induced optical rotation in oxygen-containing organic molecules*, *Physical Chemistry Chemical Physics* **25**, 27731–27743 (2023).
156. Perttu Hilla and **Juha Vaara**: *Water molecules confined in cryptophane nanocages: Structures and dynamics driven by hydrogen bonding and water chains*, *Journal of Physical Chemistry B* **128**, 3027–3036 (2024).
157. Sarah E. Mailhiot, Petri Peuravaara, Benjamin D. Egleston, Rachel J. Kearsey, Jiří Mareš, Sanna Komulainen, Anne Selent, Anu M. Kantola, Andrew I. Cooper, **Juha Vaara**, Rebecca L. Greenaway, Perttu Lantto, and Ville-Veikko Telkki: *Gas Uptake and Thermodynamics in Porous Liquids Elucidated by <sup>129</sup>Xe NMR*, *Journal of Physical Chemistry Letters* **15**, 5323–5330 (2024).
158. P. Garbacz and **J. Vaara**: *Chirality-Sensitive Effects Induced by Antisymmetric Spin-Spin Coupling*, in P. Garbacz (ed.), *Physical Principles of Chirality in NMR* (Royal Society of Chemistry, 2024), pp. 204–242.
159. Perttu Hilla and **Juha Vaara**: *Rela<sup>2</sup>x: Analytic and automatic NMR relaxation theory*, *Journal of Magnetic Resonance* **372**, 107828:1–13 (2025).

## 2. Peer-reviewed papers in press

160. Perttu Hilla and **Juha Vaara**: *Multiscale modelling of nuclear magnetisation dynamics: Spin relaxation, polarisation transfer and chemical exchange in <sup>129</sup>Xe@cryptophane(aq) structures*, *Physical Chemistry Chemical Physics*, *in press* (2025).

## 3. Submitted papers

161. Joni Eronen, Karl-Mikael Svensson, Nazmul Hossain, Vladimir Zhivonitko, **Juha Vaara** and Anu M. Kantola: *Characterization of the polarisation transfer to fluorinated pyridines in SABRE*, submitted for publication in *Physical Chemistry Chemical Physics* (2025).

## 4. Talks at international conferences

### Invited

1. **Juha Vaara**, Pekka Manninen, Perttu Lantto, and Kenneth Ruud: *Relativistic effects on magnetic resonance parameters by perturbation theory*, invited talk on Coastal Voyage in Quantum Chemistry, Tromsø-Trondheim, Norway, September 18–21, 2003.
2. **Juha Vaara**: *Magnetic and laser field effects on NMR parameters*, invited talk in Molecular Modeling Meeting, KTH Stockholm, May 26–28, 2004.

3. **Juha Vaara**, Teemu S. Pennanen, Matti Hanni, and Perttu Lantto: *Supramolecular calculations of intermolecular interaction effects on NMR parameters. Examples on liquid water and gaseous xenon*, invited talk at the 13<sup>th</sup> European Seminar on Computational Methods in Quantum Chemistry, Smolenice, Slovak Republic, September 21–29, 2005 (Abstracts, L21).
4. **Juha Vaara**: *Relativistic computations of Xe NMR*, invited talk at the conference Relativistic effects in heavy-element chemistry and physics (REHE 2007), Domaine Saint-Jacques, Ottrott, France, March 21–25, 2007 (Abstracts, IL6).
5. **Juha Vaara**: *Computational xenon NMR*, invited talk at the 4<sup>th</sup> International Symposium on Xenon NMR of Materials (XeMat 2009), Ruka, Finland, June 7–10, 2009 (Proceedings, O8).
6. **Juha Vaara**: *Computational studies of anisotropic NMR observables*, invited talk at the conference NMR in oriented phases (Tropea 2009), Tropea, Italy, October 1–5, 2009.
7. **Juha Vaara**: *Calculations of nuclear spin optical rotation*, invited talk at EuroMagNET II Quantum chemistry in strong magnetic fields (QCSMF) workshop, Toulouse, France, September 13–14, 2010.
8. **Juha Vaara**: *Relativistic calculations of nuclear spin optical rotation and chemical shift anisotropy relaxation*, invited talk at the conference Relativistic effects in heavy-element chemistry and physics (REHE 2010), Beijing, China, September 25–29, 2010 (Abstracts, IL–22).
9. **Juha Vaara**: *Chemical distinction by nuclear spin optical rotation*, invited talk at the 52<sup>nd</sup> Experimental Nuclear Magnetic Resonance Conference (52<sup>nd</sup> ENC), Pacific Grove, USA, April 10–15, 2011 (Abstracts, p. 43).
10. **Juha Vaara**: *Nuclear magneto-optic spectroscopy*, invited talk at Quantum Systems in Chemistry and Physics XVII (QSCP-XVII), Turku, Finland, August 19–25, 2012 (Abstracts, p. 26).
11. **Juha Vaara**: *Recent applications of NMR computation*, invited talk at the conference Relativistic effects in heavy-element chemistry and physics (REHE 2012), Corrientes, Argentina, September 12–17, 2012.
12. **Juha Vaara**: *Phenomenology of Nuclear Magneto-Optic Spectroscopy*, invited talk at the conference The Future of Electronic Structure Theory: Pushing Our Understanding and Limits (FUEST 2014), Sønderborg, Denmark, September 7–10, 2014.
13. **Juha Vaara**: *Nuclear magneto-optic spectroscopy*, invited plenary presentation at the 15<sup>th</sup> International Congress of Quantum Chemistry (ICQC15), Beijing, China, June 8–13, 2015.
14. Matti Hanni, Perttu Lantto, Michal Repiský, Jiří Mareš, Brian Saam, and **Juha Vaara**: *Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization*, invited talk at Molecular Properties and Computational Spectroscopy (MPCS17), Pisa, Italy, April 10–12, 2017.
15. **Juha Vaara**: *Chemical shift extremum of <sup>129</sup>Xe(aq) reveals details of hydrophobic solvation*, invited talk at Molecules in Extreme Environments, Midterm Meeting, Oslo, Norway, January 15–17, 2018.
16. **Juha Vaara**: *Computational studies on xenon NMR*, invited talk in International Xenon Symposium - XeMAT 2018, Philadelphia, USA, May 5–8, 2018.
17. **Juha Vaara**: *Computations of Small Physical Effects in Nuclear Magnetic Resonance*, invited talk at 10<sup>th</sup> Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), Tromsø, Norway, July 11–17, 2019.
18. **Juha Vaara**: *Splitting Hairs: Small Physical Effects in NMR*, invited talk at EUROISMAR 2019, Berlin, Germany, August 25–30, 2019.
19. **Juha Vaara**: *Quantum-Chemical Approach to Paramagnetic NMR*, invited talk at the Virtual Center of Magnetic Resonance conference, St. Andrews University, Scotland, June 3, 2021.

Other

20. **Juha Vaara**, Olga L. Malkina, Bernd Schimmelpfennig, Hermann Stoll, Marketá Munzarová, Vladimir G. Malkin, and Martin Kaupp: *Density-functional calculations of spin-orbit effects in nuclear shielding and electronic g-tensors*, talk presented at Quantum Systems in Chemistry and Physics V (QSCP-V), Uppsala, Sweden, April 13–18, 2000.
21. **Juha Vaara** and Pekka Pyykkö: *Magnetic field-induced quadrupole splitting in gaseous  $^{131}\text{Xe}$ : Quadratic and quartic field dependence*, talk presented at Hans Ågren Symposium in the Stockholm Environment 2000 (HASSE 2000), Villa Söderås, Lidingö, Sweden, September 30–October 1, 2000; talk presented at the 2001 Nordic NMR Symposium, Helsinki, August 26–29, 2001.
22. **Juha Vaara**: *Intermolecular effects on Xe chemical shifts*, talk presented at the final meeting of the EU/FP6 programme Understanding nanomaterials from the quantum perspective (NANOQUANT), Warsaw, Poland, March 17, 2007.
23. **Juha Vaara**, Teemu O. Pennanen, and Helmi Liimatainen: *Theory of nuclear magnetic resonance chemical shift in arbitrary electronic spin state*, talk presented at the 8<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2008), Sydney, Australia, September 14–19, 2008.
24. **Juha Vaara**: *Molecular magnetism group*, talk presented at the Symposium on Modern Methods of Quantum Chemistry, Mariapfarr, Austria, March 4–8, 2009.
25. **Juha Vaara**, Suvi Ikäläinen, and Perttu Lantto: *Nuclear magneto-optic spectroscopy*, talk presented at the 5<sup>th</sup> International Symposium on Xenon NMR of Materials (XeMat 2012), Dublin, Ireland, June 27–29, 2012 (Abstracts, T16).
26. **Juha Vaara**: *Theory of nuclear magneto-optic spectroscopy*, talk presented at the Workshop Modern Methods in Quantum Chemistry, Mariapfarr, Austria, February 24–March 1, 2013.
27. **Juha Vaara**: *Paramagnetic NMR theory interfacing experiments: Interpretation and excited states*, talk presented at the pNMR project meeting, Chamonix, France, September 7–8, 2013.
28. **Juha Vaara**, Jiří Mares, and Jyrki Rantaharju: *pNMR shift theory and relaxation simulations*, talk presented at the Workshop Modern Methods in Quantum Chemistry, Mariapfarr, Austria, February 21–24, 2014.
29. **Juha Vaara**: *Remarks on pNMR chemical shift and relaxation theory*, talk presented at the Workshop pNMR: From Rags to Riches, Prague, Czech Republic, July 4–5, 2015.
30. **Juha Vaara** and Jiří Mareš: *pNMR shieldings and couplings in the S·D·S realm*, talk presented at the Training Workshop Recent development in theory and experiment for solid-state paramagnetic NMR, Aarhus, Denmark, July 8–9, 2016.
31. **Juha Vaara**: *Paramagnetic NMR shieldings and couplings in the S·D·S realm*, talk presented in the Workshop 20<sup>th</sup> Anniversary of nuclear magnetic resonance at Luleå University of Technology, Luleå, Sweden, December 16, 2016.
32. **Juha Vaara**: *”Small” effects in NMR—Two examples of theory rationalising experimental findings*, talk presented in the 41<sup>st</sup> Danish NMR Meeting, Korsør, Denmark, January 20–21, 2020.
33. **Juha Vaara**: *Direct Enantiomeric Discrimination Through Hyperfine Coupling—A Computational Study*, talk presented at XIV<sup>th</sup> Workshop on Modern Methods in Quantum Chemistry, on-line, March 1–3, 2021.
34. **Juha Vaara**: *Multiscale Modelling of Spin Hyperpolarisation Physics*, talk presented at the XV<sup>th</sup> Workshop Modern Methods in Quantum Chemistry, Mariapfarr, Austria, February 27–March 2, 2023.
35. **Juha Vaara**: *Quantum-chemical studies in spin physics*, round-table presentation at The International Hyperpolarization Conference (HYP23), Leipzig, Germany, September 24–28, 2023.

36. **Juha Vaara**: *Polarisation transfer in spin-exchange optical pumping*, talk presented at the XVII<sup>th</sup> Workshop Modern Methods in Quantum Chemistry, Mariapfarr, Austria, February 24–28, 2025.

## 5. Talks at national conferences

1. **Juha Vaara**, Tapio T. Rantala, and Jukka Jokisaari:  *$^{21}\text{Ne}$ ,  $^{83}\text{Kr}$  and  $^{131}\text{Xe}$  NMR: A comparison of experiments with ab initio estimated relaxation rates*, talk presented at the XVI National NMR Symposium, Turku, Finland, June 3–4, 1993. Program and Abstracts, Meddelanden i serie B No. 130, Department of Organic Chemistry, Åbo Akademi University, Turku 1993.
2. **Juha Vaara**, Tapio T. Rantala, Juhani Lounila, Juha-Heikki Kantola and Jukka Jokisaari: *First principles computation of NMR parameters*, talk presented at the XVIII National NMR Symposium, Ikaalinen, Finland, June 12–14, 1996. Proceedings, Defence Forces Research Centre Publications A **10**, Ylöjärvi, 1996, p. 73–77.
3. **J. Vaara**, K. Ruud, O. Vahtras, H. Ågren, and J. Jokisaari: *Electronic spin-orbit interaction and NMR spectral parameters*, talk presented at The XXXII Annual Conference of the Finnish Physical Society, Tampere, Finland, March 19–21, 1998. Proceedings, Report 1-1998, Tampere University of Technology, Tampere 1998, 2.4.
4. **J. Vaara** and P. Pyykkö: *Magnetic field-induced quadrupole splitting in gaseous and liquid  $^{131}\text{Xe}$  NMR: Quadratic and quartic field dependence*, talk presented at the XXXV Annual Conference of the Finnish Physical Society, Jyväskylä, Finland, March 22–24, 2001. Proceedings, Research Report No. 5/2001, Department of Physics, University of Jyväskylä, Jyväskylä, 2001, 8.1.
5. **Juha Vaara** and Pekka Pyykkö: *Dirac-Fock calculations of the nuclear magnetic shielding constants of noble gas atoms*, talk presented at the XXXVI Annual Conference of the Finnish Physical Society, Joensuu, Finland, March 14–16, 2002. Proceedings, Selected Papers 7, Department of Physics, University of Joensuu, Joensuu, 2002, 8.2.
6. **J. Vaara**, Z. Rinkevicius, L. Telyatnyk, and O. Vahtras: *Non-relativistic calculations of nuclear magnetic shielding in paramagnetic molecules*, talk presented at 25<sup>th</sup> Finnish NMR Symposium, Helsinki, Finland, June 5–7, 2003. Abstracts p. 19.
7. **Juha Vaara**: *NMR parameters from quantum-chemical computation*, talk presented at the XXVII Finnish NMR Symposium, Pudasjärvi, Finland, June 8–10, 2005. Abstracts L21.
8. **Juha Vaara**, Matti Hanni, Perttu Lantto, and Michal Straka: *Computational Xenon NMR*, talk presented at the XXIX Finnish NMR Symposium, Rymättylä, Finland, June 13–15, 2007. Abstracts, p. 30.
9. **Juha Vaara**, Suvi Ikäläinen, and Perttu Lantto: *Nuclear Magneto-Optic Spectroscopy*, talk presented at the XXXIV Finnish NMR Symposium, Turku, Finland, June 13–15, 2012. Abstracts, p. 21.
10. **Juha Vaara**: *Theory of Nuclear Magneto-Optic Spectroscopy*, talk presented at the 47<sup>th</sup> Annual Conference of the Finnish Physical Society, Espoo, Finland, March 14–16, 2013.
11. **Juha Vaara**: *Theory and computation of magnetic resonance*, invited talk presented at the CECAM kick-off event, Aalto University, August 29–30, 2013.
12. **Juha Vaara**: *Phenomenology of Nuclear Magneto-Optic Spectroscopy*, talk presented at the XXXVI Finnish NMR Symposium, Pikku-Syöte, Finland, June 4–6, 2014; talk presented at the seminar on Light-Matter Interaction, Tampere University of Technology, Tampere, Finland, February 13, 2015.
13. **Juha Vaara**: *Predicting new spectroscopies: Interplay between light and nuclear magnetism*, talk presented in the Computational Chemistry Symposium of the Finnish Chemistry Days, Helsinki, Finland, March 19, 2015.

14. **J. Vaara:** *Theory and computation of magnetic resonance@Oulu*, talk presented in the XXXVIII Finnish NMR Symposium, Laukaa, Finland, June 13–15, 2016. Book of Abstracts, p. 12.
15. **Juha Vaara:** *Theory and Computation of Magnetic Resonance*, talk presented in the Computational Chemistry Day, Joensuu, Finland, August 25, 2016.
16. **Juha Vaara:** *Quantum Chemical Computation of pNMR Parameters*, invited talk presented in the Computational Chemistry Days, Helsinki, Finland, May 28–29, 2018.

## 6. Other seminars and lectures

1. **Juha Vaara:** *First principles calculation of NMR parameters*, plenary lecture at the meeting "35 Years of NMR spectroscopy at the University of Oulu", University of Oulu, Oulu, Finland, September 18, 1997.
2. **Juha Vaara:** *Computational studies on the NMR parameters of molecular probes in liquids and solids*, lecture in the seminar series "Theory and computation of NMR and ESR parameters", Linköping University, Linköping, Sweden, December 1, 1997.
3. **Juha Vaara:** *Spin-orbit contributions to NMR spectral parameters*, lecture in the seminar series "Theory and computation of NMR and ESR parameters", Linköping University, Linköping, Sweden, December 1, 1997.
4. **Juha Vaara:** *NMR parameters - comparison between experiment and first principles theory*, seminar lecture, Institute of Organic Chemistry, Polish Academy Sciences, Warsaw, Poland, January 28, 1998.
5. **Juha Vaara:** *Ab initio calculations of the spin-orbit coupling contributions to NMR shielding and spin-spin coupling tensors*, seminar lecture, Graduiertenkolleg Magnetische Resonanz, Universität Stuttgart, Stuttgart, Germany, February 8, 1999.
6. **Juha Vaara:** *Density-functional calculation of relativistic corrections to parameters of magnetic resonance spectroscopy*, talk presented at the 3<sup>rd</sup> Marie Curie Fellows' Workshop, Max-Planck-Institut für Physik, Munich, Germany, October 25–27, 1999.
7. **Juha Vaara:** *1. Kvanttikemian tutkimuksesta HY:n Kemian laitoksen Ruotsinkielisessä opetuslaboratoriossa; 2. Magneettisten resonanssispektroskopioiden (NMR ja ESR) parametrien teoria ja laskenta* (in Finnish), talk presented at the meeting of the CSC Physicists' network, CSC Scientific Computing Ltd., Espoo, December 19, 2001. *Theory and calculation of NMR and ESR parameters*, talk presented at the Soft Matter seminar series, Laboratory of Computational Engineering, Helsinki University of Technology, March 27, 2002, and in the seminar series of the Laboratory of Physical Chemistry, University of Helsinki, May 20, 2003.
8. **Juha Vaara:** *Theory and computation of magnetic resonance parameters*, talk presented at the Department of Physics, Tampere University of Technology, April 20, 2006.
9. **Juha Vaara:** *Theory of nuclear magneto-optic spectroscopy*, talk presented at the Department of Physics, Tampere University of Technology, November 26, 2010; talk presented at the Department of Chemistry and Materials Science, Aalto University, May 16, 2011.
10. **Juha Vaara:** *Molekyyli­magnetismin teoria ja laskenta* (in Finnish), talk presented at the *CSC 40 years* seminar series, University of Oulu, March 25, 2011.
11. **Juha Vaara:** *Laskennallinen molekyyli- ja materiaalfysiikka* (in Finnish), talk presented at the meeting of the physics and chemistry teachers of the Finnish universities of applied sciences, Kajaani University of Applied Sciences, May 8, 2012.
12. **Juha Vaara:** *Activities in the NMR theory group, U. Oulu and Nuclear magneto-optic spectroscopy*, talk presented at the LTU-Oulu Workshop on Rare Earth Elements, Luleå University of Technology, Sweden, June 20, 2012.

13. **Juha Vaara:** *Theory of nuclear magneto-optic spectroscopy*, talk presented at (1) Istituto per i Processi Chimico-Fisici, Consiglio Nazionale delle Ricerche, Pisa, Italy, February 22, 2013; (2) Università degli Studi di Trieste, Dipartimento di Scienze Chimiche e Farmaceutiche, Trieste, Italy, April 16, 2013, (3) Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic, April 19, 2013.
14. **Juha Vaara:** *Recent computational studies of NMR parameters*, talk presented at the Institut für Chemie, Technische Universität Berlin, Germany, April 24, 2013.
15. **Juha Vaara:** *Fysiikka, yhteiskunta, innovaatiot* (in Finnish), talk presented at the grant award ceremony of the Tauno Tönnö Fund, University of Oulu, Finland, May 3, 2013.
16. **Juha Vaara:** *Uusien ydinmagneto-optisten spektroskopioiden fenomenologiaa* (in Finnish), talk presented at the Finnish Society of Sciences and Letters, Helsinki, Finland, December 15, 2014.
17. **Juha Vaara:** *Inorganic and Physical Adventures in NMR*, talk presented at the event of retirement of Prof. Risto Laitinen, University of Oulu, Finland, January 31, 2020.

## 7. Other publications

1. **Juha Vaara:** *Two-point magnetoconductance and intermode scattering in ballistic constrictions*, Diploma thesis, University of Oulu, Department of Electrical Engineering, 1992.
2. **Juha Vaara**, Tapio T. Rantala, Juhani Lounila, Juha-Heikki Kantola, and Jukka Jokisaari: *Computational studies of NMR parameters of molecular probes in liquids and solids*, CSC News **8**, 7–9 (1996).
3. **Juha Vaara:** *Computational studies on the NMR parameters of molecular probes in liquids and solids*, Report Series in Physical Sciences No 7, University of Oulu, Department of Physical Sciences, 1997 (Ph.D. thesis).
4. **Juha Vaara:** *Theory and calculations of NMR and EPR parameters*, CSC Report on Scientific Computing 1999–2000, S. Kotila and J. Haataja, eds. (CSC - Scientific Computing Ltd, 2001), pp. 118–121.
5. H. Konschin, N. Runeberg, D. Sundholm, and **J. Vaara:** *Tarkkoja työkaluja monitieteelliseen tutkimukseen. Kansainvälinen kvanttikemian konferenssi Kuusamossa* (in Finnish), *Kemia-Kemi* **29**, 52 (2002).
6. **Juha Vaara:** *Theory and quantum-chemical calculation of magnetic resonance parameters*, CSC Report on Scientific Computing in Finland 2004–2005, J. Fagerholm, L. Puska, J. Åström, J. Blomqvist, P.-L. Forsström, L. Jukka, S. Kotila, M. M. Laine, M. Miettinen, J. Tarus, and S. Tissari, eds. (CSC -Scientific Computing Ltd, 2005), pp. 106–109.
7. **Juha Vaara:** *Laskennallinen magneettisen resonanssin tutkimus: Silta spektrien ja molekyyli mallien välillä* (in Finnish), *Tietoyhteys* 2/2006, pp. 10–12.
8. **Juha Vaara:** *Laguna maksaa, mutta myös tuottaa* (in Finnish), letter to the editor of the daily newspaper *Kaleva* (Oulu, Finland), January 3<sup>rd</sup>, 2013.
9. **Juha Vaara:** *Ydinmagneto-optisen spektroskopian fenomenologiaa* (in Finnish), *Sphinx* 2014–2015, year-book of The Finnish Society of Sciences and Letters, pp. 81–92.

Oulu, May 12, 2025, Juha Vaara