

1. Full names: Juha Tapani Vaara

2. Date and place of birth: July 7, 1967, Kemijärvi, Finland

3. Place of residence: Oulu, Finland

4. Nationality: Finnish

5. Current position

- Professor in physics, U. Oulu (UO)/Dept. Phys. (DP), 08/09–01/11. 02/11– permanent, specialisation *Computational molecular and materials physics*.
- Title of docent in physical chemistry, U. Helsinki (UH), 04/03–.
- Title of docent in physics, UO, 12/99–.

6. Education and training

- Ph.D. (filosofian tohtori), physics, UO/DP, 09/97, grade *laudatur*.
- M.Sc. (diplomi-insinööri), microelectronics and material physics, UO, Dept. of Electrical Engineering (EE), 11/92. Grade *oivallisesti*.
- High school graduation, Kemijärven lukio, 05/86. *Laudatur* ×6.

7. Research

- Theory and computation of magnetic, optical and magneto-optic properties of atoms, molecules and materials. ISI Web of Science (November 14, 2023): 157 papers, 4728 citations, *h*-index 37.

8. Previous professional appointments

- Group leader in the Finnish Center of Excellence in *Computational Molecular Science* (CMS), 01/06–12/11 (72 mo).
- UH/Dept. of Chemistry (DC). University Lecturer (yliopistonlehtori, permanent position) in physical chemistry, 08/03–01/11 (19 mo), leave of absence 08/09–01/11.
- UH/DC. Academy Research Fellow (akatemiatutkija) of the Academy of Finland, 08/02–09/07 (62 mo), Researcher 10–12/07 (3 mo).
- UH/DC. Theory of NMR and ESR parameters. Host Prof. Pekka Pyykkö, 01/00–07/02 [31 mo, of which 24 mo as Junior Research Fellow (tutkijatohtori) of the Academy of Finland].
- Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany. Spin-orbit and other relativistic effects on NMR and ESR parameters with Privatdozent Martin Kaupp, 11/98–12/99 (14 mo).
- Linköping U., Dept. of Physics and Measurement Technology, Sweden. Relativistic spin-orbit interaction contributions to NMR parameters with Prof. Hans Ågren, 1997 (3 mo).
- UO/DP. Theory and computation of NMR parameters with Docents Juhani Lounila and Tapio Rantala, as well as Prof. Jukka Jokisaari, 01/93–10/98 (total 67 mo). Nominated to the following posts: (1) assistant (asistentti) in physics 08/95–12/99; (2) senior assistant (yliasistentti) in physics 01/00–07/03.
- UO, Dept. of Theoretical Physics. Phenomenological models of high- T_c superconductors with Prof. Alpo Kallio, 1990 (3 mo).
- UO/EE, Microelectronics and Material Physics Laboratories. Experimental (1) conductance response of SnO₂ gas sensors and (2) Raman spectroscopy of diamond-like carbon films, with Profs. Vilho Lantto and Seppo Leppävuori, 1989 and 06/91–12/92 (total 23 months).

9. Research awards, research honours, and major stipendiary support for research

- EU/TMR Marie Curie Fellowship, 98–99; Vilho, Yrjö, and Kalle Väisälä Fellowship, 1999; *Doctor primus*, UO, all faculties, 05/02; membership in Suomen Tiedeseura—Societas Scientiarum Fennica, 2011; membership in Suomalainen Tiedeakatemia—Academia Scientiarum Fennica, 2021.

- Major grants after obtaining Ph.D.

1998	European Commission	ECU	68032
1999	Vilho, Yrjö and Kalle Väisälä Fund	FIM	58333
2000–05	Academy of Finland (two)	EUR	291000
2003	Emil Aaltonen Foundation	EUR	190000
2005–07	European Commission	EUR	166358
2006–11	National CoE Programme & UH	EUR	367485
2007	UH (3-year research grant)	EUR	120000
2009–11	UO (several)	EUR	115000
2010	European Commission	EUR	169888
2011–16	Academy of Finland (two)	EUR	870453
2012–13	Professor Pool (sabbatical)	EUR	25000
2013–16	European Commission	EUR	274000
2015–16	Academy of Finland	EUR	79305
2016–18	European Commission	EUR	179326
2016–20	Academy of Finland	EUR	406460
2020–24	Academy of Finland	EUR	482476
2024–27	Ministry of Education and Culture	EUR	255000
2024–28	Finnish Research Council	EUR	590908

10. Other academic and professional activities

- Postdoc supervisor for (8): Dr. Rodolfo H. Romero (UH/DC, Argentina, 03–04), Dr. Michal Straka (UH/DC, Czech Republic, 04–07), Dr. Perttu Lantto (UH/DC, Finland, 06–07), Dr. Jiří Mareš (UO/DP, Czech Republic, 09–17), Dr. Li-juan Fu (UO/DP, China, 12–14), Dr. Pär Håkansson (UO/DP, Sweden, 16–18), Dr. Karl-Mikael Svensson (UO/DP, Sweden, 21–24), Dr. Rajgowrav Cheenikundil (UO/DP, India, 25–).

- Ph.D. supervision

- Completed (13): Dr. Perttu Lantto (Ph.D., physics), UO/DP 02; Dr. Pekka Manninen (Ph.D., physics), UO/DP 04; Dr. Matti Hanni (Ph.D., physics), UO/DP 11 (co-supervisor Dr. P. Lantto); Dr. Stefan Taubert (Ph.D., physical chemistry), UH/DC 11 (as co-supervisor with Prof. D. Sundholm); Dr. Teemu O. Pennanen (Ph.D., physical chemistry), UH/DC 11; Dr. Teemu S. Pennanen (Ph.D., physics), UO/DP 11 (co-supervisor Dr. P. Lantto); Dr. Suvi Ikäläinen (Ph.D., physical chemistry), UH/DC 12; Dr. Nergiz Özcan-Ketola (Ph.D., physical chemistry), UH/DC 15; Dr. Jarkko Vähäkangas (Ph.D., physics), UO/DP 15 (co-supervisor Dr. P. Lantto); Dr. Juho Roukala (physics), UO/DP 2016 (as co-supervisor with Dr. P. Lantto); Dr. Syed Awais Rouf (Ph.D., physics), UO/NMR Spectroscopy 17 (co-supervisor Dr. J. Mareš); Dr. Jyrki Rantaharju (physics), UO/NMR Spectroscopy 19, Dr. Jouni Karjalainen (physics), UO/NMR Spectroscopy 21 (as co-supervisor with Dr. P. Lantto).
- In progress (6): Mr. Perttu Hilla (physics), UO/NMR; Ms. Megha Mohan (physics), UO/NMR (co-supervisors Prof. V.-V. Telkki and Dr. A. M. Kantola); Mr. Ari Pyykkönen (physics), UO/NMR; Mr. Joni Eronen (physics), UO/NMR (as co-supervisor with Dr. A. M. Kantola); Ms. Alina Gallardo (physics), UO/NMR; Mr. Ehsan Gholami (physics), UO/NMR.

- Undergraduate thesis supervision

- Completed (19): M.Sc. (physics) Nuha Abuzaid, UO/NMR 17; M.Sc. (physics) Matti Hanni, UO/DP 04.; B.Sc. (physics) Perttu Hilla, UO/NMR 20; M.Sc. (physics) Perttu Hilla, UO/NMR 21; M.Sc. (physical chemistry) Marja Hyvärinen, UH/DC 10; M.Sc. (physics) Suvi Ikäläinen, UH/DP 08; M.Sc. (physics) Juha-Heikki Kantola, UO/DP 98 (as co-supervisor with Docent

Tapio Rantala); M.Sc. (physics) Jouni Karjalainen, UO/DP 09 (co-supervisor: Dr. Perttu Lantto); M.Sc. (physics) Perttu Lantto, UO/DP 98; B.Sc. (physical chemistry) Helmi Liimatainen, UH/DC 09; M.Sc. (physical chemistry) Helmi Liimatainen, UH/DC 10; M.Sc. (physics) Juho Lintuvuori, UH/DP 06; M.Sc. Joni Pennanen, UO/NMR 19 (as co-supervisor with Docent Perttu Lantto); M.Sc. (physical chemistry) Teemu O. Pennanen, UH/DC 06; M.Sc. (physics) Teemu S. Pennanen, UO/DP 04; M.Sc. (theoretical physics) Jyrki Rantaharju, UO/DP 13 (co-supervisor Dr. Jiří Mareš); B.Sc. (theoretical physics) Marko Tuomela, UO/NMR 20 (with co-supervisor Dr. J. Rantaharju); M.Sc. (physics) Perttu Tuovinen, UO/NMR 19 (as co-supervisor with Docent Perttu Lantto); M.Sc. (physics) Pauli Vähäkangas, UO/NMR 20 (as co-supervisor with Docent P. Lantto); B.Sc. (physics) Eetu Hyypiö, UO/NMR 23 (as co-supervisor with Dr. Karl-Mikael Svensson).

- In progress (2): Mr. Marko Tuomela (M.Sc., theoretical physics), UO/NMR; Mr. Niko Heikkinen (M.Sc., physics, as co-supervisor with M.Sc. Perttu Hilla), UO/NMR).
- Conference organisation (7): *Finnish Symposium on Quantum Chemistry, an International Conference*, Kuusamo, Finland, 06/01, scientific and organising committees; *4th International Symposium on Xenon NMR of Materials* (XeMat 2009), Oulu, Finland, 06/09, international advisory committee; *International Congress of Quantum Chemistry* (13th ICQC), Helsinki, Finland, 06/09, local organising committee; *The XXXVI Finnish NMR Symposium*, Pikku-Syöte, Finland, 06/14, organising committee; *Physics Days 2016*, Oulu, Finland, 05/16, programme committee; *Computational Chemistry Days*, Oulu, Finland, 2023, chair of organising committee; *EUROMAR 2025*, Oulu, Finland, to be organised in 2025, scientific advisory board and local organising committee.
- Co-organisation of Winter Schools of Theoretical Chemistry, UH/DC (5): 01 *Condensed Phase Dynamics*; 02 *Large Molecules: Linear Scaling and Related Electronic Structure Calculation Methods*; 03 *Quantum Chemistry Bordering Nanoscience and Nanotechnology*; 04 *A Frontier of Chemistry: New Species*; 05 *Nanophotonics*.
- Referee activity for international scientific publications (40 different): M. Kaupp, M. Bühl, and V. G. Malkin (Eds.): *Calculation of NMR and EPR Parameters: Theory and Applications* (Wiley-VCH, 04); Chemistry-A European Journal (02–04,16); Chemical Physics (06–); ChemPhysChem (06–); Chemical Physics Letters (05–); International Journal of Quantum Chemistry (03,14); Journal of the American Chemical Society (02–); Journal of Chemical Physics (04–), Journal of Chemical Theory and Computation (08–); Journal of Computational Chemistry (06); Computational & Theoretical Chemistry (earlier Journal of Molecular Structure: THEOCHEM, 07–); Journal of Physical Chemistry (02–); Magnetic Resonance in Chemistry (04, 10, 20); Molecular Physics (03,18); Physical Chemistry Chemical Physics (07–); Physics Letters A (05); Physical Review A (08–); M. Barysz and Y. Ishikawa (Eds.): *Relativistic methods for chemists* (Springer UK, 09); Theoretical Chemistry Accounts (09–); International Reviews in Physical Chemistry (09); Physical Review E (10); Journal of Materials Chemistry (10); scientific monograph (Taylor & Francis, 10); Nature Chemistry (12); Physical Review Letters (12–); R. H. Contreras (Ed.): *High resolution nuclear magnetic resonance parameters for understanding molecules and their electronic structure* (Elsevier, Amsterdam) (2012); Journal of Applied Physics (13); Journal of Physical Chemistry Letters (14–); Arabian Journal of Chemistry (14); Nature Communications (15); Journal of Molecular Graphics and Modelling (16); Angewandte Chemie International Edition (18); Magnetochemistry (18); Carbon (19); AIP Advances (20); Applied Physics A (21); Inorganic Chemistry (22); Journal of Molecular Liquids (23); Physical Review Applied (23); Physical Review B (23–).
- Evaluation of research applications (6): Academy of Finland, 05 (evaluation panel in chemistry); Marsden Fund (New Zealand), 08 (panel in Physical sciences and engineering); EU FP7, 11 (external expert on IEF, IIF, and IOF applications); US Department of Energy, the Office for Basic Energy Sciences, 23 and 24; Agence Nationale de la Recherche (France), 23.
- Member of the national graduate schools (2): *Comput. Chemistry and Molecular Spectroscopy* (LASKEMO, 06–09); *Nanoscience* (NGS-NANO, 07–09).
- Member of the Board of the Doctoral Programme in Exact Sciences (EXACTUS DP), U. Oulu Graduate School (UniOGS, 13–14).

- Member of the Board of Directors of UO, 14–17.
- Member of the steering group of the Finnish Publication Forum (Julkaisufoorumi) appointed by the Federation of Finnish Learned Societies (Tieteellisten seurain valtuuskunta), 24–27.
- Participation in international consortia and projects (5): Marie Curie Individual Fellowship project of EU/FP6: *Computational Toolbox for Calculations of Noble Gas Magnetic Resonance Parameters* (CTNGMR, scientist-in-charge, 05–07); Marie Curie Intra-European Fellowship project of EU/FP7: *Computation of Nuclear Magnetic Relaxation in Paramagnetic Systems* (CNMRPS, scientist-in-charge, 10–12); Initial Training Network of EU/FP7: *Pushing the Envelope of Nuclear Magnetic Resonance Spectroscopy for Paramagnetic Systems. A Combined Experimental and Theoretical Approach*, (pNMR, principal investigator of the Finnish node, total of 13 nodes, 13–16); Marie Curie Intra-European Fellowship project of EU/H2020: *Quantum-Statistical Methods for Nuclear Singlet States in Complex Fluids* (QUNS, scientist-in-charge, 16–18); project *The Spectroscopy and Quantum Mechanics of C₇₀-Based Endofullerenes*, [Engineering and Physical Sciences Research Council (UK), project partner, 24–27].
- Referee for university positions (7): University researcher in phys. chem., Doc. Karoliina Honkala, U. Jyväskylä/DC, 12; title of docent in comp. chem., Dr. Krister Henriksson, UH/DC, 10; title of docent in biophysics, Dr. Oana Cramariuc, Tampere U. Technology (TUT)/DP, 13; title of docent in design of medicine, Dr. Tuomo Laitinen, U. Eastern Finland/Faculty of Health Sciences, 14; title of docent in computational physics: modelling of bio- and nanomaterials, Dr. Sami Paavilainen, TUT/DP, 16; full professor in computational physics, Prof. Jaakko Akola, TUT/DP, 17; title of docent in physical biochemistry, Dr. Vivek Sharma, UH/DP, 18.
- Faculty opponent for the following Ph.D. theses (4): Markku Leino, TUT/DP, 07; Johan Henriksson, Linköping U., Sweden, 08.; Akseli Mansikkamäki, U. Jyväskylä/DC, 18; Shehryar Khan, Stockholm U., Sweden, 18.
- Preliminary examiner of the following Ph.D. theses (20): Branislav Jansík, KTH Biotechnology, Stockholm (member of thesis committee), 04; Timo Rajamäki, UH/DC, 04; Jonas Jusélius, UH/DC, 04; Janne Hirvi, U. Joensuu/DC, 08; Ville Arpiainen, TUT/DP, 09; Andris Gulāns, Aalto U./DP, 11; Matti Viitala, TUT/DP, 11; Teemu Salmi, U. Helsinki/DC, 12; Sami Auvinen, Lappeenranta U. Technology/Dept. Mathematics and Physics, 13; Elena Heikkilä, TUT/DP, 14; Iina Juurinen, UH/DP, 14; Artur Wodyński, U. Warsaw/Chemistry, 15; Valtteri Mäkelä, UH/DC, 15; Richard Hatz, UH/DC, 15; Lauri Partanen, UH/DC, 17; Zhiwei Chang, Lund U. (member of thesis committee), 17; Matti Javanainen, TUT/DP, 18; Juha Tiihonen, U. Tampere/Physics, 19; Maria Dimitrova, UH/DC, 19; Teemu Järvinen, U. Jyväskylä/DC, 22; Vili-Taneli Salo, UH/DC, 24.
- Examiner for the following lower theses (11): Jani Saunavaara, Lic.Sc., UO/DP, 07; Tommi Virtanen, M.Sc., UH/DC, 04; Ville Weijo, M.Sc., UH/DP, 05; Ilkka Kylänpää, M.Sc., TUT/DP, 06; Artturi Koivuniemi, M.Sc., UH/DC, 06; Hanna Lignell, M.Sc., UH/DC, 08; Juho Roukala, M.Sc., UO/DP, 10; Katja Hyvönen, M.Sc., UO/DP, 15; Jari Markkanen, B.Sc., UO/NMR, 17 and M.Sc., UO/NMR, 19; Jari Havisto, B.Sc., UO/NMR, 19 and M.Sc., UO/NMR, 20.

Oulu, February 7, 2025, Juha Vaara