New method for material research gets hundred times stronger

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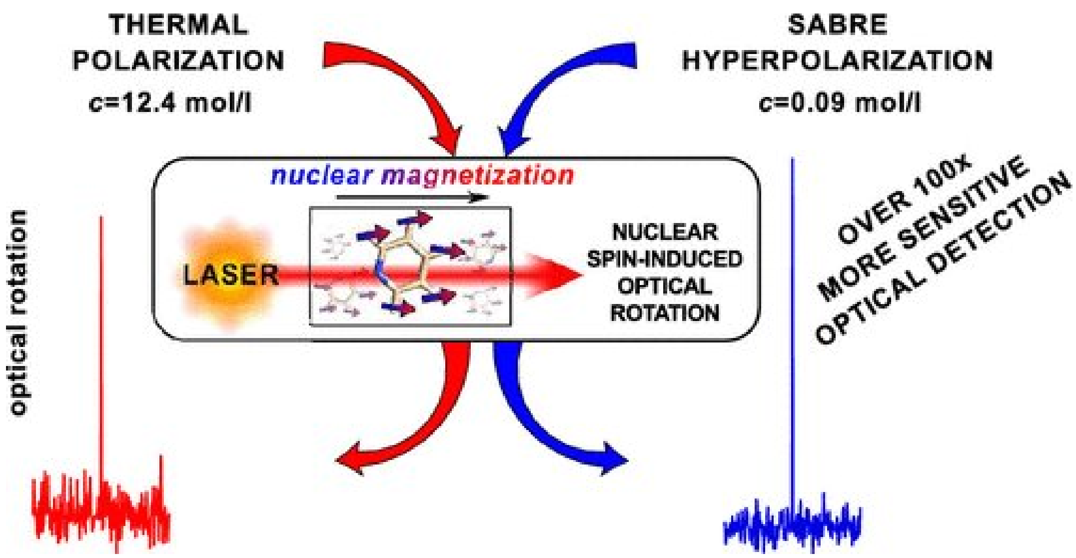

Nuclear spin-induced optical rotation (NSOR) is a promising phenomenon for molecular structure elucidation due to its sensitivity to electronic structure near atomic nuclei. It is the only experimentally verified nuclear magneto-optic effect (NMOE), so far observed usually in neat liquids or in concentrated binary mixtures, with the proportion of the minor component at least 10%. We report a method to extend the lower-concentration range of NSOR measurements by 2 orders of magnitude by employing continuous-flow SABRE (signal amplification by reversible exchange) hyperpolarization. This approach significantly increases the sensitivity of NSOR and enables its detection in dilute samples, as demonstrated with measurements of NSOR of 90 mmol/L solutions of pyridine and pyrazine. The results are compared with first-principles calculations, and good agreement is found. The possibility to measure low-concentration solutions significantly extends the pool of samples available for further studies of NMOEs. https://doi.org/10.1021/acs.jpclett.9b02194

Researchers from the Faculty of Science at the University of Oulu have increased the sensitivity of an emerging spectroscopic method with promising applications for materials studies.

All atoms that make up the ordinary matter in the Universe have nuclei, most of which behave like microscopic bar magnets. If properly oriented in space, these magnetic moments can cause small changes in the properties of light as it passes through the material, in so-called nuclear magneto-optic (NMO) phenomena. The NMO effects, first of which has been observed in 2006, enable emerging methods for studies of materials and molecules. With ability to look into the matter at the resolution of individual atoms, without permanently altering the sample properties, NMO approaches offer a valuable window into the properties of matter that only a few methods can give. In this respect, the NMO methods are similar to nuclear magnetic resonance, which is used widely in chemistry, as well as magnetic resonance imaging, an extremely powerful medical diagnostic tool.

The NMR Research Unit at the Faculty of Science has been active in the field of NMO since 2008 and has significantly contributed to the development of its theory. Lately, the group has also been involved in the development of experimental NMO techniques.

The ultimate aim of the NMO research is to provide high-sensitivity optical data with atomic-resolution about the studied material. It is crucial to improve the spectroscopic sensitivity, so that smaller samples can be measured and higher-quality information can be obtained.

The sensitivity improvement can be gained by special techniques called hyperpolarization, when the microscopic magnets of the atomic nuclei are oriented in the desired direction to a far greater degree than possible under ambient conditions. In the newest paper, published in the *Journal of Physical Chemistry Letters*, the researchers Petr Štěpánek and Anu

Kantola of the NMR Research Unit have shown how this can be achieved via the use of specially prepared hydrogen gas.

Hydrogen gas molecules can be present in two forms, the so-called ortho- and para-hydrogen, which differ by the mutual orientation of their own two nuclear magnetic moments. The high degree of orientational order contained in the gas that contains an excess of para-hydrogen, can via a catalytic reaction be transfered to the studied molecule, leading to an increase in the observed signal.

The researchers have used this method in a new combined approach and improved the sensitivity of NMO measurements by a factor of more than one hundred. This allows measurements of substances that would otherwise not be viable and opens new possibilities for further development of this new and exciting field.

More information: Petr Štěpánek et al. Low-Concentration Measurements of Nuclear Spin-Induced Optical Rotation Using SABRE Hyperpolarization, *The Journal of Physical Chemistry Letters* (2019). DOI: 10.1021/acs.jpclett.9b02194

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