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📍 Present employment: Post-doctoral researcher at Gakushuin University, Tokyo, Japan

Education

- 2014 – 2021 **Integrated Ph.D. (Masters & Ph.D. joint program), National Yang Ming Chiao Tung University**, Hsinchu, Taiwan.
Thesis title: *Standardization of Raman spectroscopy and the determination of absolute Raman cross-sections*, under Prof. Hiro-o Hamaguchi and Prof. Henryk A. Witek
- 2010 – 2013 **B.Sc. Chemistry Hons., Banaras Hindu University**, Varanasi, India.

Specialization

- 📖 **Raman Spectroscopy**, Raman intensities and cross-sections, accurate wavenumber and intensity calibration with associated data-analysis protocols
- 📖 Ro-vibrational spectroscopy of **H₂ and isotopologues** from both theoretical and experimental approaches.
- 📖 Condensed phase vibrational spectroscopy of water and hydrogen bonding

Research Publications

Journal Articles

- 1 Balashov, A. A., **Raj, A.**, Wójtewicz, S., Ciuryło, R., Lisak, D., & Bielska, K. (2024). Theoretically predicted CO₂ lines near 700 nm not observed. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 320, 108978. [doi:https://doi.org/10.1016/j.jqsrt.2024.108978](https://doi.org/10.1016/j.jqsrt.2024.108978)
- 2 Sacco, A., Mandrile, L., Tay, L.-L., Itoh, N., **Raj, A.**, Moure, A., ... Rossi, A. M. (2023). Quantification of titanium dioxide (TiO₂) anatase and rutile polymorphs in binary mixtures by Raman spectroscopy: An interlaboratory comparison. *Metrologia*, 60(5), 055011. [doi:10.1088/1681-7575/acf76d](https://doi.org/10.1088/1681-7575/acf76d)
- 3 Chen, C.-Y., Hsieh, M.-J., **Raj, A.**, Peng, W.-C., Hamaguchi, H.-o., Chuang, W.-T., ... Wang, C.-L. (2023). Missing piece in colloidal stability: morphological factor of hydrophobic nanoparticles. *Langmuir*, 39(8), 2922–2931. [doi:10.1021/acs.langmuir.2c02582](https://doi.org/10.1021/acs.langmuir.2c02582)
- 4 **Raj, A.**, Chao, Y.-B., & Witek, H. A. (2022). Testing the limitations of harmonic approximation in the determination of Raman intensities. *Molecular Physics*, e2069613. [doi:10.1080/00268976.2022.2069613](https://doi.org/10.1080/00268976.2022.2069613)
- 5 **Raj, A.**, Chen, Y.-J., Wang, C.-L., & Hamaguchi, H. (2022). Raman spectra and structure of hydrogen-bonded water oligomers in tetrahydrofuran: H₂O binary solutions. *Journal of Raman Spectroscopy*. [doi:https://doi.org/10.1002/jrs.6381](https://doi.org/10.1002/jrs.6381)
- 6 Chang, H.-Y., Wu, K.-Y., Chen, W.-C., Weng, J.-T., Chen, C.-Y., **Raj, A.**, ... Wang, C.-L. (2021). Water-induced self-assembly of amphiphilic discotic molecules for adaptive artificial water channels. *ACS Nano*, 15(9), 14885–14890. [doi:10.1021/acsnano.1c04994](https://doi.org/10.1021/acsnano.1c04994)



- 7 **Raj, A.**, Kato, C., Witek, H. A., & Hamaguchi, H. (2021). Accurate intensity calibration of multichannel spectrometers using Raman intensity ratios. *Journal of Raman Spectroscopy*, 52(12), 2038–2050. [doi:https://doi.org/10.1002/jrs.6221](https://doi.org/10.1002/jrs.6221)
- 8 **Raj, A.**, Witek, H. A., & Hamaguchi, H. (2021a). Determination of accurate absolute Raman cross-sections of benzene and cyclohexane in the gas phase. *Asian Journal of Physics*, 30, 321–335.
- 9 **Raj, A.**, Witek, H. A., & Hamaguchi, H. (2021b). Evaluating stability of a Raman spectrometer for long-time experiments. *Journal of Raman Spectroscopy*, 52(5), 1032–1047. [doi:10.1002/jrs.6085](https://doi.org/10.1002/jrs.6085)
- 10 Tiwari, M. K., Verma, A., Monika, **Raj, A.**, & Saha, S. (2021). Synthesis, structural, thermal, photophysical and vibrational spectroscopic studies of potassium-polynitrile based 3D coordination polymer. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*. [doi:10.1016/j.saa.2020.118958](https://doi.org/10.1016/j.saa.2020.118958)
- 11 Chang, W.-C., **Raj, A.**, Hiramatsu, H., Li, H.-J., Ziegler, M. S., Lin, Y., ... Liu, H.-J. (2020). Linear, mixed-valent homocatenated tri-tin complexes featuring Sn–Sn bonds. *Chemical Communications*. [doi:10.1039/d0cc02699a](https://doi.org/10.1039/d0cc02699a)
- 12 **Raj, A.**, Kato, C., Witek, H. A., & Hamaguchi, H. (2020). Toward standardization of Raman spectroscopy: Accurate wavenumber and intensity calibration using rotational Raman spectra of H₂, HD, D₂, and vibration–rotation spectrum of O₂. *Journal of Raman Spectroscopy*. [doi:10.1002/jrs.5955](https://doi.org/10.1002/jrs.5955)
- 13 Yang, Y., Chen, C. Y., Liu, D. P., **Raj, A.**, Hamaguchi, H., Qiu, H. B., ... Wang, X. S. (2020). Vesicular membrane with structured interstitial water. *The Journal of Physical Chemistry B*, 124(41), 9239–9245. [doi:10.1021/acs.jpcc.0c06678](https://doi.org/10.1021/acs.jpcc.0c06678)
- 14 Yang, Y., Zhang, H., Chen, C.-Y., Liu, D. P., **Raj, A.**, Hamaguchi, H., ... Wang, X. S. (2020). Water-mediated through-space-conjugation of aromatic groups for stimuli-responsive photoluminescence. *Giant*, 3, 100028. [doi:10.1016/j.giant.2020.100028](https://doi.org/10.1016/j.giant.2020.100028)
- 15 **Raj, A.**, Witek, H. A., & Hamaguchi, H. (2019). Vibration–rotation interactions in H₂, HD and D₂ : Centrifugal distortion factors and the derivatives of polarizability invariants. *Molecular Physics*, 118(5), e1632950. [doi:10.1080/00268976.2019.1632950](https://doi.org/10.1080/00268976.2019.1632950)
- 16 **Raj, A.**, H.Hamaguchi, & Witek, H. A. (2018). Polarizability tensor invariants of H₂, HD and D₂. *The Journal of Chemical Physics*, 148(10), 104308. [doi:10.1063/1.5011433](https://doi.org/10.1063/1.5011433)

Other contributions




Software repositories associated with peer-reviewed journal articles

- Ro-vibrational matrix elements of polarizability of H₂ and isotopologues. <https://github.com/ankit7540/H2-PolarizabilityMatrixElements>, Static and dynamic invariants of polarizability (for H₂ and isotopologues) with programs for obtaining the derivatives of these invariants. <https://github.com/ankit7540/H2-PolarizabilityDerivatives>
- Wavenumber and intensity calibration of Raman spectrometers using rotational (and ro-vibrational) transitions. <https://github.com/ankit7540/RamanSpecCalibration> <https://github.com/ankit7540/IntensityCalbr>
- Testing the limitations of harmonic approximation towards the computation of Raman intensities for a series of diatomic molecules. <https://github.com/ankit7540/Raman-Intensity-Approxmn-Test>
- Set of prgrams developed in IgorPro for data analysis pertinent to Raman spectroscopy and imaging. https://github.com/ankit7540/RamanSpec_BasicOperations

Employment History



- May 2021 – June 2023  **Post-doctoral fellow** Department of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, Taiwan
- July 2023 – present  **Post-doctoral fellow** Department of Chemistry, Faculty of Science, Gakushuin University [Presently as JSPS Fellow]

Skills




- Core  Academic research and training, \LaTeX typesetting and publishing.
- Programming  IgorPro, Python, LabVIEW, Bash-Shell.
- Instrumentation  Optical instrumentation, IR and Raman spectrometer development and time-resolved spectroscopic techniques.

Miscellaneous Experience




Invited talks

- 2018  **"Determination of accurate Raman cross-sections of fundamental organic molecules for absolutely quantitative Raman spectroscopy"**. 7th ICOPVS, BARC, Mumbai.
- 2020  **"Accurate wavenumber and intensity calibration for standardization of Raman Spectroscopy"**. 7th Asian Spectroscopy Conference (Online), NTU, Singapore.



Awards and Achievements

- 2023  **JSPS Post-doctoral fellow**, Standard post-doctoral fellowship.
- 2018  **JSPS Hope Fellow**, 10th JSPS HOPE Meeting, Yokohama, Japan.
 **Best Poster Award**, 26th International Conference on Raman Spectroscopy, Jeju, South Korea.


Overseas Research Visit


- 2015  June 12th-21st, 2015 - Visited Prof. Taka-aki Ishibashi's laboratory at Department of Chemistry, University of Tsukuba, Japan for experiments on gas phase rotational Raman spectroscopy.
- 2022  March 4th-23rd, 2022 - Visited Prof. Satyen Saha's laboratory at Department of Chemistry, Banaras Hindu University, Varanasi, India for discussion on future collaborations and experiments.
- 2023  January 2nd-14th, 2023 - Visited Department of Physics under Prof. K. Bielska to perform experiments on cavity ringdown spectroscopy and design new experiments on H₂.


Poster presentations

- 2016  **"Determination of Raman cross sections for absolutely quantitative Raman spectroscopy"**. Taiwan International Symposium on Raman Spectroscopy 2016, Taipei, Taiwan.
-  **"Breath analysis with Raman spectroscopy"**. Japan-Taiwan Medical Spectroscopy International Symposium (JTMSIS) 2016, Awaji Island, Japan.


Miscellaneous Experience (continued)


- 2017  **"Accurate band area estimation using a restricted summation approach based on Lebesgue integral"**. Taiwan International Symposium on Raman Spectroscopy 2017, Chiayi, Taiwan.


- 2018  **"Determination of accurate absolute Raman cross sections of benzene and other fundamental organic molecules"**. 10th JSPS HOPE Meeting 2018, Yokohama, Japan.

-  **"Determination of accurate absolute Raman cross sections of benzene and other fundamental organic molecules"**. 26th ICORS-2018, Jeju, Korea.

Academic service

- 2017–  **Peer reviewer**, Journal of Raman Spectroscopy, Wiley

- 2022–  **Peer reviewer**, Analytical Methods, RSC

- 2024–  **Peer reviewer**, Applied Spectroscopy, Sage Publication