Dr. Aloke Das
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Research Area

- Gas phase laser spectroscopy, Non-covalent interactions in biomolecules
- The major focus of the research group is on molecular level understanding of various weak non-covalent interactions which govern the structures as well as the functions of biomolecules and materials.
- They employ isolated gas phase laser spectroscopy techniques combined with quantum chemistry calculations to obtain intrinsic knowledge on the physical nature, strength, and binding motifs of these weak interactions.
- Lab is equipped with mass elected Resonant 2-Photon Ionization (R2PI) and IR-UV double resonance spectroscopy in a home-built spectrometer coupled with supersonic jet-cooling, laser desorption, resonantly enhanced multi photon ionization and Time of Flight mass spectrometry. Quantum chemistry calculations are exploited to interpret the data obtained from gas phase spectroscopy.

Profile

Education & scientific career

Aloke Das obtained his PhD degree from Indian Institute of Technology Kanpur in 2002 under the supervision of Professor Tapas Chakraborty. Subsequently, he moved to Purdue University for doing his postdoctoral research with Professor Timothy S. Zwier (2002-2004). Later, he was a post-doctoral fellow with Professor Erwin D. Poliakoff at the Louisiana State University to study Vacuum-Ultraviolet (VUV) photoelectron spectroscopy using synchrotron radiation at the Advanced Light Source of the Lawrence Berkeley National Laboratory (2004-2007).

Publications

Mishra, K. K., Borish, K., Singh, G., Panwaria, P., Metya, S., Madhusudhan, M. S.* and Das, A.* (2021). Observation of an unusually large IR red-shift in an unconventional S-H…S hydrogen bond. The Journal of Physical Chemistry Letters, 12: 1228-1235.

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Kumar, S., Mishra, K. K., Singh, S. K., Borish, K., Dey, S., Sarkar, B.* and Das, A.* (2019). Observation of a weak intra-residue C5 hydrogen-bond in a dipeptide containing Gly-Pro sequence. The Journal of Chemical Physics, 151: 104309-8.

Mishra, K. K., Singh, S. K., Kumar, S., Singh, G., Sarkar, B.*, Madhusudhan, M. S.* and Das, A.* (2019). Watermediated selenium hydrogen-bonding in proteins: PDB analysis and gas phase spectroscopy of model complexes. The Journal of Physical Chemistry A, 123: 5995-6002.

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Deb, P., Jin, G. Y., Singh, S. K., Moon, J., Kwon, H., Das, A.*, Bagchi, S.* and Kim, Y. S.* (2018) Interconverting hydrogen bonding and weak n→π* Interactions in aqueous solution: A direct spectroscopic evidence. The Journal of Physical Chemistry Letters, 9: 5425-5429.

Mishra, K. K., Singh, S. K., Ghosh, P., Ghosh, D.* and Das, A.* (2017). The nature of selenium hydrogen bonding: gas phase spectroscopy and quantum chemistry calculations. Physical Chemistry Chemical Physics, 19: 24179-24187.

Singh, S. K., Mishra, K. K., Sharma, N. and Das, A.* (2016). Direct spectroscopic evidence for an n→π*
interaction. Angewandte Chemie International Edition, 55: 7801-7805.

Singh, S. K., and Das, A.* (2015). n→π* interaction: A rapidly emerging non-covalent interaction. Physical Chemistry Chemical Physics, 17: 9596-9612.