RIE BHOPAL, Faculty Profile (Last five years from 2019-2025)

<table>
<tr><td>Full Name:</td><td colspan="3">Dr. MANOJ MANDAL</td><td rowspan="5">  </td></tr>
<tr><td>Designation:</td><td colspan="3">Assistant Professor</td></tr>
<tr><td>Department:</td><td colspan="3">Department of Education in Science and Mathematics (Chemistry Section)</td></tr>
<tr><td>Official Address:</td><td colspan="3">Regional Institute of Education, National Council of Educational Research and Training, Shyamla Hills, Bhopal – 462002, Madhya Pradesh, India</td></tr>
<tr><td>Telephone:</td><td></td><td>Fax:</td><td>---</td></tr>
<tr><td>Mobile:</td><td colspan="4">9123909866</td></tr>
<tr><td>Email:</td><td colspan="4">mandalmanojcu@gmail.com, manoj.mandal@ncert.nic.in</td></tr>
<tr><td colspan="2">Education Qualification:</td><td colspan="3">M. Sc., Ph.D., Post-doc</td></tr>
<tr><td colspan="2">Teaching Experience:</td><td>02 yrs</td><td>Research Experience:</td><td>09 yrs (post Ph.D.)</td></tr>
</table>

Academic Identity:

(i) ORCID Id with web link: https://orcid.org/0000-0003-0184-3168

(ii) Scopus Author Id with web link:

https://www.scopus.com/authid/detail.uri?authorId=56229902000

(iii) Researcher Institutional ID with web link

(iv) Google Scholar Id with web link:

https://scholar.google.com/citations?user=wXAKErcAAAAJ&hl=en

(v) Vidwan Id: with web link: https://vidwan.inflibnet.ac.in/profile/620542

(vi) Research gate Id with web link:

Research Interest and Fields of Specialization

- Theoretical and Computational Chemistry
- Atomistic and Multiscale molecular modelling
- Protein structure, function, and dynamics
- Natural and artificial photosynthesis
- Enzyme catalysis
- Protein – drug interaction
- Chemistry Education

Member of Academic Institutions (Board of Studies / Research Degree Committee/School Board) Present/ Past

1. **Membership of different Organizations:** NA

2. Research Supervision
   (No. of Ph.D. Degree Awarded_____0_____ and Registered_____0_____)

   (Number of M.Phil awarded in _____0_____)

3. **Research Projects (Completed and ongoing with title, type, fund allocated, duration and name of the funding agency):**
   Title: "Exploring the water-oxidation mechanism and proton coupled electron transfer reactions in photosystem II: an approach towards clean fuel"
   PI: Dr. Manoj Mandal
   Fund allocated: Rs.1,13,60,000/-
   Duration: 15/07/2021 to 14/07/2026
   Funding agency: Department of Biotechnology, Ministry of Science and Technology, Govt. of India.

4. **Administrative Experience:** 01 yr

5. **Scientific Visits Abroad/ International Collaboration:**

   The University of Tokyo, Tokyo, Japan (January, 2019 – December, 2020)
   Postdoctoral Researcher

6. **Conference/Symposium/Workshop Attended during (2019-2025)**

- Invited talk at NCL Pune on 28th July, 2023.
  - **Title:** *Proton coupled electron transfer reactions during natural water oxidation in photosystem II*
- Invited talk at IISER Pune on 27th July, 2023.
  - **Title:** *Why nature choose redox-active low barrier H-bonds in photosystem II?*
- Invited talk in a tropical research school on "The recent trends of research in theoretical and experimental physics" from 20-23 March, 2023 at Gurucharan College, Silchar, Assam.
  - **Title:** *Applications of physics and chemistry in biology*
- Invited talk at IISC Bangalore on16th January, 2023.
  - **Title:** Water oxidation mechanism and proton coupled electron transfer reactions in photosystem II
- Invited talk in a conference on "Recent Advances in Chemistry: Theoretical and Computational Aspects 2022" jointly organized by NIT Meghalaya and NEHU, November 18-20, 2022, Shillong.
  - **Title:** *Role of low-barrier H-bond in proton coupled electron transfer reactions*
- Theoretical Chemistry Meeting: Structure and Dynamics (TCMSD-2022), 26th to 29th May, 2022, IACS, Kolkata (Poster)
- The 46th Symposium on Biomolecular Science, 2019, University of Tsukuba, Japan
  - **Title:** *Water-splitting mechanism of photosystem II and ammonia binding sites near oxygen evolving complex.*

- International Conference on artificial photosynthesis-2019(ICARP2019), 2019, Hiroshima, Japan (Poster)

7. A) **Research Papers Published in Journals last six years (2019-2025) (Include H-Index, i10 Index and total No of Citation as Per Scopus/Google Scholar):**

The format of Publication details should include: Authors Name (as appeared in the journal), Title of the Paper, Name of the Journal with ISSN no, Volume, Page No, DOI:___, Year of Publication, Publisher Name, Country of Publication, Indexed, in: Scopus/Web of Science.

H-Index: 11
i10 Index: 11
Total No of Citation: 290

1. Manoj Mandal*, Keisuke Saito, Hiroshi Ishikita*
"Substitution of Ca^{2+} and changes in H-bond network near the oxygen evolving complex of photosystem II"
Phys. Chem. Chem. Phys., 25, 6473-6480, 2023, ISSN: 1463-9084
DOI: 10.1039/D2CP05036F
The Royal Society of Chemistry (RSC); United Kingdom, Web of Science.

2. Manoj Mandal, Keisuke Saito, Hiroshi Ishikita*
"Release of the proton and formation of the low-barrier hydrogen bond between tyrosine D and D2-His189 in photosystem II"
ACS Physical Chemistry Au, 2, 423-429, 2022. ISSN: 2694-2445
DOI: 10.1021/acsphyschemau.2c00019
American Chemical Society (ACS), USA, Web of Science

3. Manoj Mandal, Keisuke Saito, Hiroshi Ishikita*
"Release of Electrons and Protons from Substrate Water Molecules at the Oxygen-Evolving Complex in Photosystem II"
J. Phys. Soc. Jpn., 91, 091012, 2022, ISSN: 1347-4073
DOI: 10.7566/JPSJ.91.091012
Physical Society of Japan (JPS), Japan, Web of Science

4. Manoj Mandal, Keisuke Saito, Hiroshi Ishikita*
"Requirement of Chloride for the Downhill Electron Transfer Pathway from the Water-Splitting Center in Natural Photosynthesis"
J. Phys. Chem. B, 126, 123-131, 2022, ISSN: 1520-6106
DOI: 10.1021/acs.jpcb.1c09176
American Chemical Society (ACS), USA, Web of Science

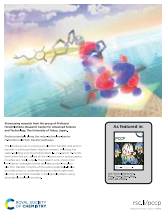
5. Keisuke Saito*, Minesato Nakagawa, Manoj Mandal, Hiroshi Ishikita*
"Role of redox-inactive metals in controlling the redox potential of heterometallic manganese-oxido clusters"
Photosynthesis Research, 148, 153-159, 2021, ISSN: 1573-5079
DOI: 10.1007/s11120-021-00846-y
Springer Nature, The Netherlands, Web of Science

6. Divya Kaur, Yingying Zhang, Krystle M. Reiss, Manoj Mandal, Gary W. Brudvig, Victor S. Batistac, M.R. Gunner*
"Proton exit pathways surrounding the oxygen evolving complex of photosystem II"
BBA - Bioenergetics, 1862, 148446, 2021, ISSN: 0005-2728
DOI: 10.1016/j.bbabio.2021.148446
Elsevier, The Netherlands, Web of Science

7. Manoj Mandal, Keisuke Saito, Hiroshi Ishikita*
"Two Distinct Oxygen-Radical Conformations in the X-ray Free Electron Laser Structures of Photosystem II"
J. Phys. Chem. Lett., 12, 4032-4037, 2021, ISSN: 1948-7185
DOI: 10.1021/acs.jpclett.1c00814
American Chemical Society (ACS), USA, Web of Science

8. Manoj Mandal, Keisuke Saito, and Hiroshi Ishikita*
"The Nature of the Short Oxygen-Oxygen Distance in the Mn_4CaO_6 Complex of the Photosystem II Crystals"
J. Phys. Chem. Lett., 11, 10262-10268, 2020, ISSN: 1948-7185
DOI: 10.1021/acs.jpclett.0c02868
American Chemical Society (ACS), USA, Web of Science
[Remarks - Cover Article]

9. Keisuke Saito†, Manoj Mandal†, and Hiroshi Ishikita* (Remarks: †Joint first authors)
"Redox potentials along the redox-active low-barrier H-bonds in electron transfer pathways"
Phys. Chem. Chem. Phys., 22, 25467, 2020, ISSN: 1463-9084
DOI: 10.1039/d0cp04265j
The Royal Society of Chemistry (RSC); United Kingdom, Web of Science.
[Remarks – Back Cover Article]



10. Keisuke Saito, Manoj Mandal, and Hiroshi Ishikita*
"Energetics of ionized water molecules in the H-bond network near the Ca^{2+} and Cl^- binding sites in photosystem II"
Biochemistry, 59, 3216, 2020, ISSN: 0006-2960
DOI: 10.1021/acs.biochem.0c00177
American Chemical Society (ACS), USA, Web of Science
[Remarks - Cover Article]

11. Manoj Mandal, Keisuke Kawashima, Keisuke Saito, and Hiroshi Ishikita*
"Redox Potential of the Oxygen-Evolving Complex in the Electron Transfer Cascade of Photosystem II"
J. Phys. Chem. Lett., 11, 249, 2020, ISSN: 1948-7185
DOI: 10.1021/acs.jpclett.9b02831
American Chemical Society (ACS), USA, Web of Science
[Remarks - Cover Article]

12. Manoj Mandal, Atanu Das*, and Chaitali Mukhopadhyay*
"Ubiquitin Folds via a Flip-Twist-Lock Mechanism"
BBA-Proteins and Proteomics, 2020, 1868, 140299, ISSN:1878-1454
DOI: 10.1016/j.bbapap.2019.140299
Elsevier, The Netherlands, Web of Science

13. Divya Kaur, Xiuhong Cai, Umesh Khaniya, Yingying Zhang, Junjun Mao, Manoj Mandal and Marilyn R. Gunner*
"Tracing the Pathways of Waters and Protons in Photosystem II and Cytochrome c Oxidase"
Inorganics,7, 14, 2019, ISSN: 2304-6740
DOI: 10.3390/inorganics7020014
MDPI, Switzerland, Web of Science

B) ARTICLES PUBLISHED IN THE EDITED BOOK : NA

C) PAPER PUBLISHED (IN CONFERENCE PROCEEDING with ISSN Number): NA

D) PUBLICATION OF BOOKS (Both as Authored and Edited): NA

E) PREPARATION OF STUDY MATERIAL: NA

F) EDITORSHIP OF RESEARCH JOURNAL: NA

G) MOOCs: NA

8) ORGANIZATION of SEMINAR/WORKSHOP/FDP/TRAING PROGRAM: NA

9) Other Information if any:

Served as a reviewer for prestigious peer-reviewed international journals:

(a) The journal of physical chemistry letters
(b) The journal of physical chemistry
(c) Biochemistry
(d) ACS Omega
etc.