

## Curriculum vitae

### Personal profile:

First name : Krishna Reddy Tel: +49-89 289 13462 (Lab)  
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Date of birth : January 1, 1988  
Gender : Male  
Marital status : Married  
Nationality : Indian  
Languages known : English, Telugu and German  
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Permanant address : S/o Nandipati Venkata Reddy, 2-41, Mandapam bajar, Konanki,  
Guntur, Piduguralla, Andhra Pradesh, 522413, India

### Education:

- Ph.D. (November 30, 2017)  
University of Hyderabad, Hyderabad, India.  
Thesis title: **Control of chemical dynamics by IR and UV laser pulses.**  
Supervisor: Prof. Susanta Mahapatra
- Master's degree. (Chemical Sciences) (2011)  
Grade points: 7.2/10, First class. University of Hyderabad, Hyderabad, India.  
Master's project title: **Collision induced dissociation dynamics of  $\text{Li}+\text{H}_2^+$  reaction.**
- Bachelor's degree (Maths, Physics, Chemistry as major subjects) (2008)  
Aggregate: 78%, First class. SS&N College, Narasaraopet.  
Affiliated to Acharya Nagarjuna University, Andhra Pradesh, India.
- Grade 12 (2005)  
Aggregate: 92.4%, Distinction. Saradha Junior College, Narasaraopet  
Affiliated to State Board of Intermediate Education, Andhra Pradesh, India
- Grade 10 (2003)  
Aggregate: 90.4%, Distinction. Z P High School, Tummalacheruvu.  
Affiliated to Board of Secondary Education, Andhra Pradesh, India.

### Current & past employment:

- Postdoc (Dec 05, 2019- present)  
Heidelberg University, Heidelberg, Germany (Advisor: Prof. Dr. Oriol Vendrell)
- Postdoc (Dec 05, 2017- Dec 04, 2019)  
Technical University of Munich, Munich, Germany (Advisor: Prof. Dr. Wolfgang Domcke)

### Research experience/abilities:

My research interests span quantum chemistry, quantum dynamics and spectroscopy of molecular systems. In particular, I have got strong experience in quantum dynamics/spectroscopy simulations through the construction of *ab initio* models during my two postdoctoral positions in the renowned groups of Prof. Wolfgang Domcke (TU Munich, Germany) and Prof. Oriol Vendrell (Heidelberg University, Germany). Below is the list of research projects that contributed to my research skills and list of research publications in peer-reviewed scientific journals that demonstrate my research abilities.

## A. List of research projects:

- Worked as a research assistant in computational studies of high-energy materials (May-October, 2009), ACRHEM, University of Hyderabad.
- Worked on a reactive scattering dynamics project titled '**Collision induced dissociation dynamics of  $\text{Li}+\text{H}_2^+$  reaction**' in Master's degree (January-June, 2011).
- Worked on 'Optimal laser-controlled dynamics' project in PhD (2012-2017) and guided a master thesis in this field
- Worked on DFG sponsored project 'Jahn-Teller dynamics of transition metal tetrafluorides' in Prof. Domcke's group (December, 2017-November, 2019).
- Currently working on a DFG sponsored project 'Electronic currents in ring shaped molecules induced by polarized laser pulses' in Prof. Oriol's group (December, 2019 - present).

## B. List of research publications:

1. K. R. Nandipati\* and K. A. Kumar, Optimal control of vibrational transitions of HCl, *Pramana - J. Phys.* **87**, 50 (2016).
2. K. R. Nandipati, H. Singh, S. Nagaprasad Reddy, K. A. Kumar and S. Mahapatra\*, Optimal initiation of electronic excited state mediated intramolecular H-transfer in malonaldehyde by UV-laser pulses, *Eur. Phys. J. D* **68**, 355 (2014).
3. K. R. Nandipati, K. A. Kumar, Z. Lan, H. Singh and S. Mahapatra\*, Initial state-specific photodissociation dynamics of pyrrole via  $\pi\sigma^*/S_0$  conical intersection initiated with optimally controlled UV-laser pulses, *Eur. Phys. J. D* **71**, 222 (2017).
4. K. R. Nandipati, Z. Lan, H. Singh and S. Mahapatra\*, An alternative laser driven photodissociation mechanism of pyrrole via  $\pi\sigma^*/S_0$  conical intersection, *J. Chem. Phys.* **146**, 214304 (2017).
5. K. R. Nandipati, K. A. Kumar, Z. Lan and S. Mahapatra\*, Controlled H-transfer in malonaldehyde in the electronic ground state mediated through conical intersection of  $n\pi^*$  and  $\pi\pi^*$  electronic excited states, *Phys. Chem. Chem. Phys.* **21**, 20018 (2019).
6. K. R. Nandipati\*, O. A. Vasilyev, I. S. Navarkin, V. G. Solomonik and W. Domcke, First-principles study of large-amplitude dynamic Jahn-Teller effects in vanadium tetrafluoride, *J. Chem. Phys.* **152**, 094304 (2020).
7. K. R. Nandipati\* and O. Vendrell\*, On the generation of electronic ring currents under vibronic coupling effects, *J. Chem. Phys.* **153**, 224308 (2020).
8. O. A. Vasilyev, K. R. Nandipati\*, I. S. Navarkin, V. G. Solomonik and W. Domcke, Strong static and dynamic Jahn-Teller and pseudo Jahn-Teller effects in Niobium tetrafluoride, *J. Chem. Phys.* **154**, 124305 (2021).
9. K. R. Nandipati\*, and O. Vendrell\*, Dynamical Jahn-Teller effects on the generation of electronic ring currents by circularly polarized light, *Phys. Rev. Research* **3**, L042003 (2021).
10. K. R. Nandipati\*, and O. Vendrell\*, Jahn-Teller twist on cavity-photon polarization in molecular polaritons, (to be communicated soon).

11. K. R. Nandipati, S. Sasmal and O. Vendrell, Ring currents using tight-binding Hamiltonians: application to benzene and triazine (in preparation).

(\* indicates corresponding author)

#### Scientific meetings attended/contributed to:

- Participated in **ICTS-School on Frontiers in Light-Matter interactions December 8-18, 2015**, IACS, Kolkata, India.
- Oral presentation in **Current Trends in Computational Natural Sciences, March 20, 2016**, IIIT-H, Hyderabad, India. Title of the talk: *Control of photodissociation dynamics of pyrrole*.
- Presented poster in **Theoretical Chemistry Symposium, December 14-17, 2016**, University of Hyderabad, Hyderabad, India. Poster title: *Photodissociation dynamics of pyrrole: An alternative mechanism driven by optimally controlled laser pulse*.
- Oral presentation in **QUTIF Young Researcher Meeting 2018, December 4-7**, Max-Born Institute, Berlin, Germany, Title of the talk: *An alternative laser-driven photodissociation mechanism of pyrrole*.
- Presented poster in **The XXIV<sup>th</sup> International Symposium on the Jahn-Teller Effect, June 24-29, 2018**, University of Cantabria, Santander, Spain. Poster title: *First-principles studies of Jahn-Teller effects in vanadium tetrafluoride*.
- Participated in the CECAM school **From quantum to classical molecular dynamics, May 20-24, 2019**, Saclay, Paris.
- Presented poster in **55th Symposium on Theoretical Chemistry (STC2019), September 22-26, 2019**, University of Rostock, Rostock, Germany. Poster title: *Ab initio studies of large-amplitude Jahn-Teller effects in vanadium and niobium tetrafluorides*.

#### Teaching experience/abilities:

During my PhD at the University of Hyderabad, I had the opportunity to take up the following teaching assistantships/direct courses at the Master's level:

- Teaching assistantship for the courses Quantum Mechanics and Computational Chemistry during graduate studies at University of Hyderabad.
- Teaching assistantship for the Numerical Methods and Computer Programming course at the University of Hyderabad.
- Taught Quantum Mechanics in Karnataka Central University as a Guest faculty (Oct-Nov, 2017).

In addition, my postdoctoral research on Jahn-Teller effects in molecular systems developed my competence to teach a course on Symmetry, Group theory and Spectroscopy. Overall, my training and research experience qualify me to teach the following courses: (a) Atomic and Molecular Structure and (b) Symmetry, Group theory and Spectroscopy and (c) Practical Computational Quantum Chemistry.

#### Awarded fellowships & other qualifications:

- Awarded Wenner-Gren postdoctoral fellowship (2020) to work on the project “X-ray spectroscopy of dynamic Stark effects at conical intersections in molecules”, at the Royal Institute of Technology (KTH) Stockholm, Sweden.

- Awarded Council of Scientific and Industrial Research (CSIR, India) - junior and senior research fellowships (December, 2011- December, 2016) for carrying out PhD at the University of Hyderabad. Overall rank obtained in the CSIR conducted National Eligibility Test (NET) was 69 (National rank).
- Qualified Graduate Aptitude Test in Engineering (GATE, 2011) for admission into PhD program in Indian Institute of Technologies.
- Qualified University of Hyderabad National level M.Sc. entrance examination (2009-June) (National rank 13) for getting admission into Master's degree at the School of Chemistry, University of Hyderabad.
- Computer skills: Fortran & Python languages, MCTDH, Gaussian, Mopac, Molpro etc.

### **Referees:**

1. Prof. Susanta Mahapatra  
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2. Prof. Dr. Wolfgang Domcke  
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3. Prof. Dr. Oriol Vendrell  
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