

**Curriculum formativo, didattico, scientifico e professionale del candidato**

**Dichiarazione sostitutiva di certificazioni**

(Art. 46, D.P.R. 28 dicembre 2000 n. 445)

**Dichiarazione sostitutiva dell'atto di notorietà**

(da sottoscrivere davanti all'impiegato addetto o da presentare o spedire con la fotocopia di un documento di identità)

(Art. 47, D.P.R. 28 dicembre 2000 n. 445)

Estremi del bando di selezione	SELEZIONE PER L'ATTRIBUZIONE DI N. 1 BORSA DI RICERCA DAL TITOLO: "Sviluppo degli applicativi per il calcolo di forme e volumi di siti di legame proteici e di molecole all'interno del progetto "Take the (bi)cycle: a new computational pipeline for transformative screening and design of (bi)cyclic peptides." – Responsabile scientifico prof. Attilio Vittorio Vargiu	
Informazioni aggiornate al	17/12/2025	
Nome e Cognome	Hardik Lalitkumar KAGDADA	
Data di nascita	09/02/2023	

Si raccomanda di indicare con precisione tutti gli elementi valutabili ai sensi del bando di selezione (aggiungere o togliere righe secondo necessità).

**Esperienza professionale**

Periodo	Ente	Principali attività e responsabilità
15/01/2019-15/01/2022	Teaching Assistantship	Physics Tutorials, Physics Lab duties, Departmental work (Exam supervision duties)

**Istruzione, formazione (es. titoli di studio, certificazioni professionali/linguistiche/informatiche)**

Data	Titolo / Principali tematiche	Ente
09/02/2023	Ph.D.	Ph.D. in Physics
2016	Master of Science (M.Sc.)	M.Sc. in Physics
2014	Bachelor of Science (B.Sc.)	B.Sc. in Physics

**Publicazioni / Convegni**

**Journal articles**

- Hardik L. Kagdada**, and Ankit Jain, Anomalous phonon thermal transport in boron chalcogenides: Role of four-phonon scattering. *Journal of Applied Physics*, **137**, 025106 (2025).
- Amit K. Bhojani, **Hardik L. Kagdada** and Dheeraj K. Singh. Anomalous Behavior of Lattice Thermal Conductivity in Two-Dimensional Carbon Chalcogenides. *Physical Review B*, **111**, 085419 (2025).
- Hardik L Kagdada**, and Ankit Jain, Impact of Vacancy Defects on Electrochemical Nitrogen Reduction Reaction Performance of MXenes. *ChemPhysChem*, **25**, e202300993 (2024).
- Amit K. Bhojani, **Hardik L. Kagdada** and Dheeraj K. Singh. "Ultrahigh power factor and excellent solar efficiency in two-dimensional hexagonal group-IV–V nanomaterials."

*Journal of Applied Physics*, **135**, 095106 (2024).

5. **Hardik L. Kagdada**, Basant Roondhe, Vaishali Roondhe, Shweta D. Dabhi, Wei Luo, Dheeraj K. Singh and Rajeev Ahuja. Exploring A-Site Cation Variations in Dion–Jacobson Two-Dimensional Halide Perovskites for Enhanced Solar Cell Applications: A Density Functional Theory Study, *Advanced Energy & Sustainability Research*, 2300147 (2023).
6. Amit K Bhojani, **Hardik L. Kagdada**, Rajeev Ahuja and Dheeraj K. Singh. Carbon-based Monochalcogenides for Efficient Solar and Heat Energy Harvesting, *Applied Surface Science*, **608**, 155121 (2023).
7. **Hardik L Kagdada**, Shovit Bhattacharya, Arnulf Materny and Dheeraj K Singh. Two-dimensional Halide Perovskite Materials Featuring 2-(Methylthio)ethylamine Organic Spacers for Efficient Solar and Heat Energy Harvesting, *Journal of Physical Chemistry C*, **126**, 21518-21526 (2022).
8. **Hardik L Kagdada**, Arnulf Materny and Dheeraj K Singh. Decreasing Toxicity and Increasing Photoconversion Efficiency by Sn-substitution of Pb in 5-ammonium Valeric Acid-based Two-dimensional Hybrid Perovskite Materials, *Physical Chemistry Chemical Physics*, **24**, 23226-23235 (2022). [Featured as 2022 PCCP HOT Article]
9. Deepak K. Pandey, **Hardik L. Kagdada**, Arnulf Materny, and Dheeraj K. Singh. "Adsorption and breaking of hazardous methyl mercury on hybrid structures of ionic liquids and ZnO nanoclusters." *Journal of Molecular Liquids*, **364**, 19957 (2022).
10. **Hardik L. Kagdada**, Sanjeev K. Gupta, Satyaprakash Sahoo, and Dheeraj K. Singh. "Mobility Driven Thermoelectric and Optical Properties of Two-Dimensional Halide-based Hybrid Perovskites: Impact of Organic Cation Rotation." *Physical Chemistry Chemical Physics*, **24**, 8867 (2022).
11. Vishakha Kaushik,\* **Hardik L. Kagdada,\*** Dheeraj K. Singh, Sachin Pathak "Enhancement of SERS effect in Graphene-Silver hybrids." *Applied Surface Science*, **574**, 151724 (2022). (\*Contributed equally)
12. Paridhi Sanchora, Deepak K. Pandey, **Hardik L. Kagdada**, and Dheeraj K. Singh "Understanding the fundamental interaction mechanism of hazardous gases and imidazolium based ionic liquids for efficient gas adsorption." *Chemical Engineering Science*, **247**, 117031 (2022)
13. Deepak K. Pandey, **Hardik L. Kagdada**, Arnulf Materny, and Dheeraj K. Singh. "Hybrid Structure of Ionic Liquid and TiO<sub>2</sub> Nanoclusters for Efficient Hydrogen Evolution Reaction." *The Journal of Physical Chemistry A*, **125**, 2653-2665 (2021).
14. Deepak K. Pandey, **Hardik L. Kagdada**, Arnulf Materny, and Dheeraj K. Singh. "Hybrid Structure of Ionic Liquid and ZnO Nano Clusters for Potential Application in Dye-Sensitized Solar Cells." *Journal of Molecular Liquids*, **322**, 114538 (2021).
15. **Hardik L. Kagdada**, Sanjeev K. Gupta, Satyaprakash Sahoo, and Dheeraj K. Singh. "Rashba Splitting in Two Dimensional Hybrid Perovskite Materials for High Efficient Solar and Heat Energy Harvesting." *Journal of Physical Chemistry Letters*, **11**, 7679-7686 (2020).
16. **Hardik L. Kagdada**, Prafulla K. Jha, Piotr Śpiewak, Krzysztof J. Kurzydłowski, and Dheeraj K. Singh. "Pressure-induced First Order Phase Transition in Bulk GeSe." *Journal of*

*Applied Physics*, **127**, 175104 (2020).

17. Paridhi Sanchora, Deepak K. Pandey, **Hardik L. Kagdada**, Arnulf Materny, and Dheeraj K. Singh. "Impact of Alkyl Chain Length and Water on The Structure and Properties of 1-Alkyl-3-Methylimidazolium Chloride Ionic Liquids." *Physical Chemistry Chemical Physics*, **22**, 17687-17704 (2020).
18. Basant Roondhe, Vaishali Sharma, **Hardik L. Kagdada**, Dheeraj K. Singh, Tanusri Saha Dasgupta, and Rajeev Ahuja. "Enhancing the Electronic and Phonon Transport Properties of Two-Dimensional Hexagonal Boron Nitride Through Oxygenation: A First Principles Study." *Applied Surface Science*, **533** 147513 (2020).
19. Vaishali Sharma, **Hardik L. Kagdada**, Jinlan Wang, and Prafulla K. Jha. "Hydrogen Adsorption on Pristine and Platinum Decorated Graphene Quantum Dot: A First Principle Study." *International Journal of Hydrogen Energy*, **45**, 23977-23987 (2020).
20. Vaishali Sharma, **Hardik L. Kagdada**, and Prafulla K. Jha. "Four-Fold Enhancement in the Thermoelectric Power Factor of Germanium Selenide Monolayer by Adsorption of Graphene Quantum Dot." *Energy*, **196**, 117104 (2020).
21. **Hardik L. Kagdada**, Shweta D. Dabhi, Venu Mankad, Satyam M. Shinde, and Prafulla K. Jha. "First Principles Study on Small  $ZrAl_n$  and  $HfAl_n$  Clusters: Structural, Stability, Electronic States and  $CO_2$  Adsorption." *Materials Chemistry and Physics*, **239**, 122264 (2020).
22. Vaishali Sharma, **Hardik L. Kagdada**, Prafulla K. Jha, Piotr Śpiewak, and Krzysztof J. Kurzydłowski. "Halogenation of SiGe Monolayers: Robust Changes in Electronic and Thermal Transport." *Physical Chemistry Chemical Physics*, **21**, 19488-19498 (2019).
23. **Hardik L. Kagdada**, Prafulla K. Jha, Piotr Śpiewak, and Krzysztof J. Kurzydłowski. "Understanding the Behavior of Electronic and Phonon Transports in Germanium Based Two Dimensional Chalcogenides." *Journal of Applied Physics*, **124**, 235701 (2018).
24. **Hardik L. Kagdada**, Shweta D. Dabhi, and Prafulla K. Jha. "Density Functional Study of Adsorption and Desorption Dynamics of Hydrogen in Zirconium Doped Aluminium Clusters." *International Journal of Hydrogen Energy*, **43**, 21724-21731 (2018).
25. **Hardik L. Kagdada**, Prafulla K. Jha, Piotr Śpiewak, and Krzysztof J. Kurzydłowski. "Structural Stability, Dynamical Stability, Thermoelectric Properties, and Elastic Properties of GeTe at High Pressure." *Physical Review B*, **97**, 134105 (2018).

### Review Articles

1. Vaishali Sharma, **Hardik L. Kagdada**, Prafulla K. Jha, Piotr Śpiewak, and Krzysztof J. Kurzydłowski. "Thermal Transport Properties of Boron Nitride Based Materials: A Review." *Renewable and Sustainable Energy Reviews*, **120**, 109622 (2020).

### Conference Proceedings

1. **Hardik L. Kagdada**, Vaishali Sharma, Prafulla K. Jha, and Dheeraj K. Singh. "Strain Induced Enhancement in Thermoelectric Power Factor of  $ZrTe_2$ " *AIP Conference Proceedings*, **2265**, 030463, AIP Publishing LLC, 2020.
2. **Hardik L. Kagdada**, Anjali Patel, and Prafulla K. Jha. "Structural, Magnetic and

Electronic Properties of Ferrimagnetic and Non-Magnetic Cubic Phase of  $MnV_2O_4$ " *AIP Conference Proceedings*, **2115**, 030486. AIP Publishing LLC, 2019.

3. **Hardik L. Kagdada**, Shweta D. Dabhi, and Prafulla K. Jha. "Bandgap Tuning and Enhancement of Seebeck Coefficient in One Dimensional GeSe." In *AIP Conference Proceedings*, **1942**, 110010, AIP Publishing LLC, 2018.

### Book Chapters

1. **Hardik L. Kagdada**, Vaishali Sharma, Ajit Kumar Parwani, and Dheeraj K. Singh. Strain-Engineered Electronic and Thermoelectric Properties of Two-Dimensional SnGe. In *Recent Advances in Mechanical Infrastructure*, pp. 59-67. Springer, Singapore, 2022
2. Deepak K Pandey, **Hardik L Kagdada**, Paridhi Sanchora, Dheeraj K Singh. "Overview of Raman Spectroscopy: Fundamental to Applications", In *Modern Techniques of Spectroscopy: Basics, Instrumentation, and Applications*, pp. 145-184. Springer, Singapore, 2021.
3. Vaishali Sharma, **Hardik L. Kagdada**, Dheeraj K. Singh, and Prafulla K. Jha. "Trapping Melamine with Pristine and Functionalized Graphene Quantum Dots: DFT and SERS Studies." In *Advances in Spectroscopy: Molecules to Materials*, pp. 441-451. Springer, Singapore, 2019.
4. **Hardik L. Kagdada**, Hiral J. Trivedi, Sharad B. Pillai, Narayan N. Som, and Prafulla K. Jha. "Structural, Electronic and Dynamical Properties of Binary Alloy Zr-Al Using Density Functional Theory." In *Advanced Materials Research*, vol. 1141, pp. 204-209. Trans Tech Publications Ltd, 2016.

### Altre attività scientifiche

#### Invited Talks/Conference/Seminar/workshops attended

- Participated and present work in FisMat 2025 conference held at the Ca' Foscari University, Venice (7–11 July, 2025)

**Oral Presentation:** Thermal Transport in Metal Oxide Frameworks: Lattice Dynamics and Electron-phonon Coupling Approach

- Participated and presented two posters in the **European Materials Research Society EMRS Spring Meeting 2024** (EMRS-2024) spring meeting organized at Strasbourg, France (26-31 May, 2024).

**Poster Presentation:** Impact of Vacancy Defects on Electrochemical Nitrogen Reduction Reaction Performance of MXenes

**Poster Presentation:** Exploring A-site Cation Variations in Dion-Jacobson Two-Dimensional Halide Perovskites for Enhanced Solar Cell Applications: A DFT Study

- Participated and presented work in "College on Energy Transport and Energy Conversion in the Quantum Regime" held at The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy (12- 30 August 2019)

**Short Invited Talk:** *Halogenation of SiGe monolayer: Robust change in electronic and thermal transport*

**Poster Presentation:** *Enhancement of Thermoelectric Figure of Merit by Quantum*

### *Confinement Effect in Germanium Telluride (GeTe)*

- ❑ Online International Conference on Recent Advances in Functional Materials (RAFM-2022) organized by Department of Physics, IQAC, ARSD college, University of Delhi, on 14-16 March 2022. **Awarded by Best Oral Presentation**

**Oral Presentation:** *Rashba Splitting in Two Dimensional Hybrid Perovskite Materials for High Efficient Solar and Heat Energy Harvesting*

- ❑ Online Workshop on Excited Charge Dynamics in Semiconductors, organized by The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy (28-30 Sept. 2020)
- ❑ E-Conference (webinar) on “Leveraging Science and Technology to Combat COVID-19” organized by Faculty of Science, DDU Gorakhpur University, Gorakhpur (23-24 May 2020)
- ❑ 64<sup>th</sup> DAE Solid State Physics Symposium held at Indian Institute of Technology Jodhpur, India (18-22 Dec 2019)

**Poster Presentation:** *Strain induced enhancement in thermoelectric power factor of ZrTe<sub>2</sub>*

- ❑ 63<sup>rd</sup> DAE Solid State Physics Symposium held at Guru Jambheshwar University of Science & Technology, Hisar, India (18-22<sup>nd</sup> Dec 2018)

**Poster Presentation:** *Structural, magnetic and electronic properties of ferrimagnetic and non-magnetic cubic phase of MnV<sub>2</sub>O<sub>4</sub>*

- ❑ 62<sup>nd</sup> DAE Solid State Physics Symposium held at DAE Convention Centre, Bhabha Atomic Research Centre (BARC), Mumbai, India, (26-30<sup>th</sup> Dec 2017)

**Poster Presentation:** *Bandgap tuning and enhancement of Seebeck coefficient in one dimensional GeSe*

- ❑ “Recent Trends on Membranes and Separation Technology (RTMST)” held at CSMCRI-Bhavnagar, Gujarat during 22-23 Nov. 2017

**Poster Presentation:** *Density Functional Study of Adsorption and Desorption of Hydrogen on Zirconium Doped Aluminium Clusters*

- ❑ 6<sup>th</sup> International Conference on Perspective in Vibrational Spectroscopy (ICOPVS 2016) held at the University of Lucknow, Lucknow from 5-8 Nov. 2016.

- ❑ Got the Opportunity to do a 2-month project as a Summer Fellow on “*Study of Cloud Base Height over Ahmedabad*” at Physical Research Laboratory, Ahmedabad, from 16<sup>th</sup> May to 8 July 2016.

- ❑ Participated in an open house and Science fair and demonstrated a model of “Simple Electric Train” at The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat on 3<sup>rd</sup> and 4<sup>th</sup> January 2016

- ❑ Presented a poster entitled “*Structural, electronic and dynamical properties of binary alloy Zr-Al using density functional theory*” in NCSM-2K15 held at The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat on December 28 – 30, 2015.

### **Ulteriori informazioni pertinenti**

#### **Technical Skills**

- **High-performance computing:** CPUs & GPUs (SpaceTime – IITB, PARAM, CLAMV – Germany, ICM – Poland)
- **Simulation codes:** Quantum Espresso, Gaussian16, GPUMD, LAMMPS, VASP, ShengBTE

- **Data analysis:** ASE, Matplotlib, Origin, Gnuplot, VESTA, Xcrysden, Gaussview
- **Programming:** Python, bash scripts, C/C++
- **Operating Systems:** Ubuntu, CentOS, Windows

Luogo, data e firma

Cagliari, il 17/12/2025

Digitally signed by Hardik  
Kagdada

