ALLEGATO B

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: "Caratterizzazione termoelettrica di sistemi metal-organic frameworks bidimensionali e a layer tramite simulazioni atomistiche ab initio" – Responsabile scientifico dott. Riccardo Dettori
Informazioni aggiornate al	30/03/2026
Nome e Cognome	Hardik Lalitkumar KAGDADA
Data di nascita	

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**
01/2025-12/2025	Postdoctoral researcher	Research work (electronic transport properties)
03/2023 – 12/2024	Institute Postdoctoral Fellow	Research work (thermal transport and electrochemical reactions), Lab and Exam supervision duties
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	Bachlor of Science (B.Sc.)	B.Sc. in Physics

Pubblicazioni / Convegni

Journal articles

1. Neha Rajput, Nidheesh Virakante, **Hardik L. Kagdada,** Ankit Jain, Thermal transport properties of diamond and hard carbon allotrope using machine-learning driven atomistic simulations. *Computational Materials Science,* **268,** 114648 (2026),
2. **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).
3. 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).

4. **Hardik L Kagdada**, and Ankit Jain, Impact of Vacancy Defects on Electrochemical Nitrogen Reduction Reaction Performance of MXenes. *ChemPhysChem,* **25,** e202300993 (2024).
5. 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).
6. **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).
7. 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).
8. **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).
9. **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**]
10. 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).
11. **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).
12. 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)
13. 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)
14. Deepak K. Pandey, **Hardik L. Kagdada,** Arnulf Materny, and Dheeraj K. Singh. "Hybrid Structure of Ionic Liquid and TiO_2 Nanoclusters for Efficient Hydrogen Evolution Reaction." *The Journal of Physical Chemistry A*, **125,** 2653-2665 (2021).
15. 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).

16. **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).
17. **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).
18. 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).
19. 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).
20. 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).
21. 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).
22. **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).
23. 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).
24. **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).
25. **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).
26. **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)
- ❒ 64th 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* $ZrTe_2$
- ❒ 63rd DAE Solid State Physics Symposium held at Guru Jambheswar University of Science & Technology, Hisar, India (18-22nd Dec 2018)

  Poster Presentation: *Structural, magnetic and electronic properties of ferrimagnetic and non-magnetic cubic phase of* MnV_2O_4
- ❒ 62nd DAE Solid State Physics Symposium held at DAE Convention Centre, Bhabha Atomic Research Centre (BARC), Mumbai, India, (26-30th 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*
- ❒ 6th 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 16th 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 3rd and 4th 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

• **Simulation methods:** First-principles calculations, lattice dynamics, electronic and thermoelectric properties, Boltztrap transport theory.

• **High-performance computing:** CPUs & GPUs (SpaceTime – IITB, PARAM, CLAMV – Germany, ICM – Poland)

• **Simulation codes:** Quantum Espresso, Gaussian16, GPUMD, LAMMPS, VASP, Phonopy, ShengBTE

• **Data analysis:** ASE, Matplotlib, Origin, Gnuplot, VESTA, Xcrysden, Gaussview

• **Programming:** Python, bash scripts

• **Operating Systems:** Ubuntu, CentOS, Windows

Luogo, data e firma

Cagl` `ri, il 30/03/2026