Review Report on PhD Thesis

Faculty: Central European Institute of Technology
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Student: Krishna Sampathkumar
Doctoral Study Program: Advanced Materials and Nanosciences
Field of Study: Advanced Nanotechnologies and Microtechnologies
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The thesis delves into an advanced topic of nanomaterials, namely strain engineering in 2D materials such as graphene and transition metal dichalcogenides (TMDs) to control their properties. The study is notable because of its potential uses in flexible electronics, optoelectronics, and energy systems. The thesis makes a significant contribution to tackling important difficulties in the field of 2D materials by incorporating machine learning for material characterisation and employing modern experimental methodologies.
The topicality stems from its multidisciplinary approach, which combines experimental physics, materials science, and computational methods (ML) to discover novel physical phenomena and propose answers for practical applications. This integration emphasizes the thesis's relevance to growing developments in sustainable technology and advanced materials. The emphasis is on developing scalable and efficient technologies, such as polymer swelling for strain induction.

Meeting the Goals Set

The stated objectives, which include the development of sample preparation techniques, strain-induced property modulation, and the use of machine learning, have been fully met. The experimental findings are well supported by theoretical ideas, and the thesis follows a logical path from problem formulation to solution creation.

Problem Solving and Dissertation Results:

- The candidate addresses key challenges in the field with remarkable rigor:
- Sample Fabrication: Developed and optimized dry transfer techniques for fabricating suspended and supported heterostructures.

- ✓ Machine Learning in Raman Analysis: The integration of advanced ML models demonstrates the potential to automate and enhance the accuracy of material characterization.
- ✓ Graphene Wrinkle Patterns: Innovative utilization of graphene wrinkles for nano-patterning opens pathways for applications like surface-enhanced Raman spectroscopy.

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- ✓ Strain-Chemical Functionalization: The analysis of strain-modulated functionalization expands the understanding of doping and surface chemistry in 2D materials.
- ✓ Biaxial Strain Effects on TMDs: Detailed studies on how biaxial strain can be imposed using the polymer swelling technique and influences their respective property was probed using the Raman, PL, and fluorescence technique provide new insights into material behavior.

These results are not only of academic significance but also have potential implications for the electronics and photonics industries.

Importance for Practice or Development of the Discipline:

The thesis bridges the gap between fundamental science and applied research, presenting a roadmap for leveraging strain engineering and machine learning in real-world applications. Key contributions include: Enhancing the simplified and precision of 2D material preparation techniques for laboratory experiments. Understanding of exciton dynamics under strain, crucial for optoelectronic devices. Establishing machine learning as a tool for robust, automated material analysis. Providing insights into the interplay of mechanical deformation and chemical functionalization, relevant for sensing and catalysis. These findings hold promise for innovations in areas such as flexible electronics, advanced sensors, and sustainable energy solutions.

Formal Adjustments and Language Level:

The thesis is well-structured, with a logical flow between chapters. The language is clear and precise, making complex concepts accessible. Minor areas for improvement include the lack of conclusion at the end of each part of experimental results and missing details such as explaining the experimental results in the polymer swelling experiments.

Questions and Comments:

- ✓ (p.35-38) Does the twist angle and related moire pattern impacts the mechanical stability of suspended heterostructures? Are they stable during long-term experiments?
- ✓ (p.39,43-45) Did the ML models account for noise introduced by variations in Raman spectral intensity across different setups? If so, how?
- ✓ (p.46) Could the sensitivity of Raman spectroscopy to strain and defects be further enhanced using advanced ML techniques?
- ✓ (p.58-61) Were there challenges in ensuring uniform wrinkle formation across large samples?
- ✓ What strategies were used to mitigate variability?
- ✓ (p.69) Could the observed increase in reactivity under strain be attributed to specific changes in graphene's electronic structure without damaging its crystallinity in both uniaxial and biaxial strain cases?

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- ✓ Beyond diazonium salts, what other functionalization strategies could benefit from strain engineering?
- ✓ (p.72) How could the findings on strain-induced exciton dynamics be translated into practical applications like photovoltaics?
- ✓ (p.74-76) How does environmental exposure (e.g., humidity, temperature) affect the stability of strain-induced exciton dynamics in TMDs? What are the mechanical limits of the polymer swelling technique in achieving higher strain levels? The description of polymer swelling-induced strain lacks detail about reproducibility and long-term stability. Could the author discuss potential limitations and mitigation strategies?
- ✓ What are the candidate's planed for extending this research into multi-functional heterostructures or quantum devices?

The thesis **by Krishna Sampathkumar** represents a significant contribution to the field of nanotechnology and advanced materials. It combines experimental ingenuity with computational innovation to address fundamental and applied challenges in 2D material science. The comprehensive exploration of strain engineering, combined with cutting-edge machine learning techniques, underscores the candidate's potential as a leading researcher in the field.

The work fulfills all requirements for obtaining a PhD degree and is ready to be defended orally before the respective committee.

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