

Paul-Drude-Institut für Festkörperelektronik (PDI) - Computational Material Science



PDI is a research institute in Berlin, Germany. We perform basic and applied research at the nexus of materials science, condensed matter physics, and device engineering.

Diamond in a Drop: Modeling Low-Pressure Growth in Liquid Metals

Master Thesis Topic, Computational Material Science

City: Berlin; Starting date (earliest): At the earliest possible; Remuneration: 13,90€/hour; Closing date: 31/03/26

Tasks

Why Diamond Matters

Diamond Isn't Just for Jewelry — It's the Future of Quantum Tech!

From quantum sensors to qubits, diamond's unmatched properties — extreme hardness, biocompatibility radiation resistance, and record-breaking thermal conductivity — make it a superstar material for next-gen technologies. But growing diamond sustainably, and at low pressure, is a game-changer. This thesis explores how carbon atoms turn into diamonds in liquid metal systems, using atomistic simulations to uncover the atomic magic behind a process that could reshape the future of quantum materials.

Your Mission

- Study how carbon behaves in molten metal alloys (Ga-Fe-Ni-Si) at moderate temperatures and atmospheric pressure.
- Explore key factors (supersaturation, bonding, surface effects) that control the formation of diamond (sp^3) vs. graphite (sp^2).
- Provide theoretical insights to guide experimental efforts in low-pressure diamond synthesis with liquid metal catalysts.

Expected Outcomes

- A validated atomistic simulation workflow for modeling carbon transport and nucleation in molten metal systems.
- Practical recommendations (a "growth recipe") for enhancing low-pressure, seed-

free diamond
growth with liquid metal catalysts.

- Potential contribution to a peer-reviewed publication and poster presentation on key findings.

Skills You'll build

- DFT Calculations: Learn to perform density functional theory calculations to analyze material behaviors.
- Molecular Dynamics Simulations: Gain hands-on experience running simulations to study atomic and molecular dynamics.
- Experience with Supercomputers: Utilize high-performance computing (HPC) systems to run large-scale simulations
- Scientific Communication: Develop the ability to present and publish your research findings in a professional context.
- Collaborative Research: Work in a collaborative environment that fosters teamwork and idea-sharing.

Requirements

Your Profile

- Bachelor's degree in materials science, physics, or a related field
- (Optional) Background in Programming skill using such as Python and familiarity with Linux/Unix environments
- Effective communication skills in english and a genuine enthusiasm for contributing to cutting-edge research in the field of materials science.

What we offer

Opportunities and Benefits

- Unique theory/simulation capabilities
- Modern laboratories with a wide range of experimental techniques
- Supportive environment with experts for various scientific sub-fields
- International and culturally diverse community
- Location in the heart of Berlin with excellent public transport connections, a subsidized travel ticket
- Possibility to participate in professional development programs

Application

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More information at <https://stellenticket.de/201887/TUB/>
Offer visible until 26/03/26

