



Universität Hamburg

DER FORSCHUNG | DER LEHRE | DER BILDUNG

Bachelorthesis

Optimization of the Quantum Espresso Density Functional Theory Code for parallel execution on the PHYSnet-Cluster

Optimierung des Quantum Espresso Dichte-Funktional Theorie
Codes für die parallele Ausführung auf dem PHYSnet-Cluster

vorgelegt von

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Kurzzusammenfassung

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Motivation

Conventions

Throughout the text of this thesis scalars are written in italic s , and vectors in bold italic \boldsymbol{v} .

I Conclusion

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