



# High-throughput All-Electron Density Functional Theory Simulations for a Data-driven Chemical Interpretation of X-ray Photoelectron Spectra

Jens Bröder

Schlüsseltechnologien / Key Technologies

Band / Volume 229

ISBN 978-3-95806-526-0

Forschungszentrum Jülich GmbH  
Peter Grünberg Institut (PGI)  
Quanten-Theorie der Materialien (PGI-1/IAS-1)

# **High-throughput All-Electron Density Functional Theory Simulations for a Data-driven Chemical Interpretation of X-ray Photoelectron Spectra**

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Schriften des Forschungszentrums Jülich  
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 229

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ISSN 1866-1807

ISBN 978-3-95806-526-0

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ISBN 978-3-95806-526-0

Mitglied der Helmholtz-Gemeinschaft

