



## The electronic structure of transition metal dichalcogenides investigated by angle-resolved photoemission spectroscopy

Mathias Gehlmann

Schlüsseltechnologien / Key Technologies  
Band / Volume 170  
ISBN 978-3-95806-324-2

Forschungszentrum Jülich GmbH  
Peter Grünberg Institut (PGI)  
Elektronische Eigenschaften (PGI-6)

# **The electronic structure of transition metal dichalcogenides investigated by angle-resolved photoemission spectroscopy**

Mathias Gehlmann

Schriften des Forschungszentrums Jülich  
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 170

---

ISSN 1866-1807

ISBN 978-3-95806-324-2

# Contents

<b>Zusammenfassung</b>	<b>1</b>
<b>Abstract</b>	<b>3</b>
<b>1 Introduction</b>	<b>5</b>
<b>2 Theoretical background</b>	<b>9</b>
2.1 Electronic band structure . . . . .	9
2.2 Spin-orbit coupling in solids . . . . .	13
2.3 Density functional theory . . . . .	16
2.3.1 The Kohn-Sham equations . . . . .	16
2.3.2 Numeric band structure calculations . . . . .	17
2.4 Photoemission spectroscopy . . . . .	20
2.4.1 The photoemission process . . . . .	20
2.4.2 Angle-resolved photoemission spectroscopy . . . . .	23
2.5 Van der Waals materials . . . . .	31
2.5.1 The van der Waals interaction . . . . .	31
2.5.2 Layered crystals . . . . .	32
2.5.3 Atomically thin materials . . . . .	33
2.5.4 Transition metal dichalcogenides . . . . .	33
<b>3 Experimental setup</b>	<b>35</b>
3.1 ARPES setup at PGI-6 . . . . .	37
3.2 Beamline 5 at DELTA . . . . .	46
3.3 Momentum microscope at Elettra . . . . .	53
<b>4 The hidden spin-polarization of 2H-MoS<sub>2</sub></b>	<b>59</b>
4.1 Sample Properties . . . . .	60
4.1.1 2H-MoS <sub>2</sub> crystal structure . . . . .	60
4.1.2 Cleavage behavior . . . . .	61

## *Contents*

---

4.1.3	Identification of the correct MoS <sub>2</sub> polytype . . . . .	63
4.2	2D electronic states in a 3D crystal . . . . .	65
4.2.1	Comparison to a freestanding monolayer . . . . .	65
4.2.2	The valence band splitting at the $\bar{K}$ point . . . . .	69
4.2.3	Surface electronic structure . . . . .	71
4.2.4	Exclusion of the 3R phase . . . . .	73
4.3	The hidden spin-polarization . . . . .	75
4.3.1	Quantum mechanical considerations . . . . .	75
4.3.2	Spin-ARPES experiments . . . . .	78
4.3.3	The initial band polarization . . . . .	81
4.3.4	Spin-layer locking . . . . .	84
4.4	Conclusions . . . . .	86
<b>5</b>	<b>The electronic structure of ReS<sub>2</sub></b>	<b>87</b>
5.1	3D band mapping ReS <sub>2</sub> bulk single crystals . . . . .	87
5.1.1	ARPES experiments and DFT calculations . . . . .	88
5.1.2	Applying the FEFS model . . . . .	94
5.1.3	Identification of the valence band maximum . . . . .	97
5.2	Atomically thin ReS <sub>2</sub> . . . . .	100
5.2.1	Sample properties . . . . .	100
5.2.2	Micro-ARPES experiments . . . . .	101
5.3	Conclusions . . . . .	106
<b>6</b>	<b>Summary and outlook</b>	<b>107</b>
<b>List of Abbreviations</b>		<b>I</b>
<b>Bibliography</b>		<b>III</b>

Schlüsseltechnologien / Key Technologies  
Band / Volume 170  
ISBN 978-3-95806-324-2