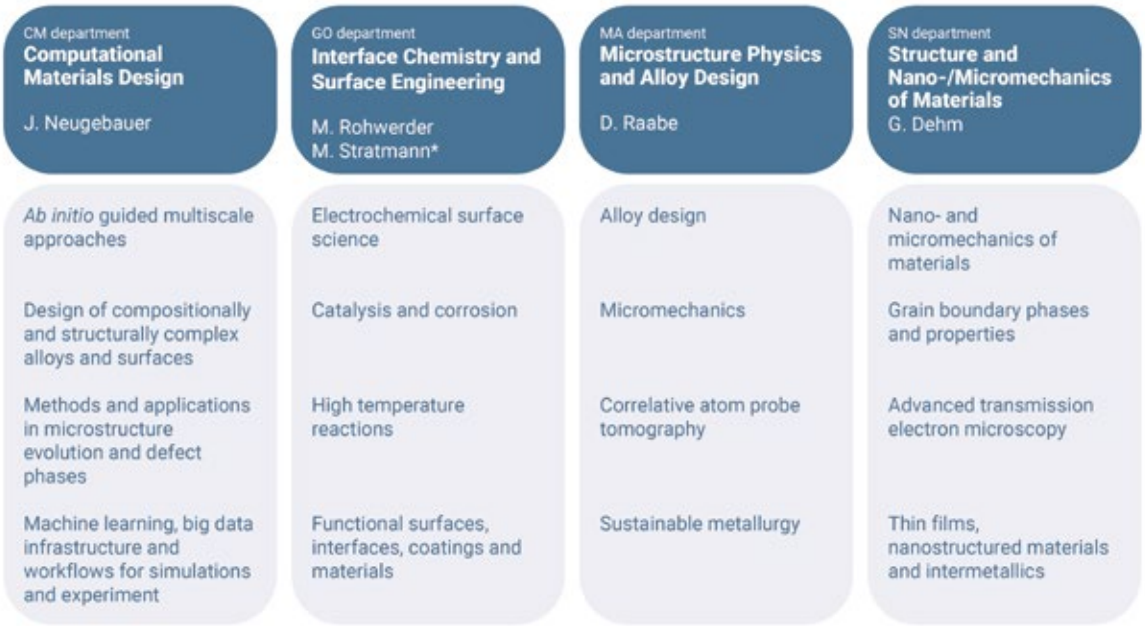
Preface

This report presents the scientific activities and achievements of the Max-Planck-Institut für Eisenforschung GmbH (MPIE) between 2019 and 2021.

The institute has four departments: Computational Materials Design (Prof. J. Neugebauer), Interface Chemistry and Surface Engineering (Prof. M. Stratmann (on leave, provisional head: Prof. J. Neugebauer)), Microstructure Physics and Alloy Design (Prof. D. Raabe) and Structure and Nano-/Micromechanics of Materials (Prof. G. Dehm). The MPIE also hosts an Independent Max Planck Research Group on Nanoanalytics and Interfaces (Prof. C. Scheu). Each department consists of several research groups. The MPIE has a number of interdepartmental and partner groups where topics of interdisciplinary content are jointly pursued. Service groups support the scientific departments. These include the synthesis, processing and testing of materials, chemical analysis, metallography, a mechanical workshop, facilities to design and build scientific equipment, an electronic workshop, a library, a computer network centre and a research coordination office.

The MPIE's mission is to understand and design materials for structural and functional applications down to atomic and electronic scales, fully including the impact of real environments. Using latest analysis methods and theory, many of them developed in-house, we start to resolve and quantify material complexity in terms of its rich nano-cosmos, manifested by hierarchical and entangled atomic-scale structural and electrochemical building units and defects. Accessing this complexity at a fundamental level is highly challenging and requires the constant development of experimental and theoretical techniques as most of the constituting nano-features are buried in the bulk, change over time (4D materials) and experience entanglements with correlations that range from a few atomic distances to several micrometres. The structural complexity of advanced materials requires also huge efforts in probing how such materials respond to external or internal chemical, physical, bio-medical and mechanical stimuli.

This mission is nowadays more essential than ever: global society enters from the age of industry into the age of circular economy, sustainability and digitalization. Advanced materials have a fundamental impact on all these fields. They can solve many of the challenges by enabling products with new features and properties. Their synthesis and manufacturing can be revolutionized by knowledge-driven workflows that integrate theory, data-driven rapid maturation and robotic production. Materials also stand for some of the most pressing burdens of our generation: Since their production causes about 50 % of all industrial CO_2 emissions and 10 % of the global energy consumption, research in this field is a matter of highest urgency.



*M. Stratmann is on leave for the time of his presidency of the Max Planck Society. J. Neugebauer is the provisional head of the department.

Fig. 1: *Scientific scopes of the departments.*

At the MPIE we address and solve many of these challenges with novel materials, functions and processes, using interdisciplinary approaches, involving experimentalists and theoreticians from different groups and departments. The often multi-disciplinary research tasks have also motivated us to found dedicated interdepartmental research groups, to foster collaboration between the different fields. Some grand research challenges that we pursue are:

— How can materials endure hydrogen exposure; what are the links between hydrogen embrittlement, alloy chemistry and microstructure? How can hydrogen ingress be prevented or tolerated?

— How can mutually exclusive properties be reconciled in a single material system?

— What is the interplay between structure, chemistry, thermodynamics and kinetics at buried lattice defects?

— How can materials heal themselves, be more adaptive to changing environments, alter their properties on demand and maintain or even improve their response under harsh system conditions?

— How can theory- and data-driven material design methods in combination with synthesis robots and automated experimental characterization enable autonomous materials discovery, synthesis and manufacturing?

— How can basic materials science help to make the entire materials system ecologically more responsible and more sustainable, serve a circular economy and break the conventional end-of life view with practically endless recycling by proper design of materials and processes?

Some recent developments are worth to be mentioned: as of Jan.1st, 2022 the MPIE has finalized its transition into 100% ownership by the Max Planck Society, while remaining its legal entity as a GmbH until administrative processes are aligned during the next years. During the past 3 years, MPIE has used the transition phase to sharpen its research profile by adding topics related to fuels cells, hydrogen, magnetism, thermoelectrics, sustainability and machine learning to its portfolio, flanked by (bi-)weekly workshops and joint seminars, including extramural partner groups.

The MPIE also participates in several large network programs amongst others 6 collaborative research centers (SFBs) funded by the German Research Foundation (DFG) and it hosts 4 ERC grants in the reporting period (in total 7 ERC Grantees since 2012). The MPIE won in 2017 and 2020 highest ranks in the Humboldt ranking among all non-university research organizations in Germany (rank 1 in engineering, rank 3 over all sciences) with 33 awarded scholarships between 2019 and 2021.

In 2020, Dr. Baptiste Gault received the highest German research award - the Gottfried Wilhelm Leibniz Award 2020 by the German Research Foundation. Over the past 3 years more than 20 members of the MPIE gained professorships from prestigious universities around the globe, underlining the institute's ambition to propel careers. And the MPIE heads the International Max Planck Research School - IMPRS SurMat.

The institute evolved not only scientifically, also work & life at the institute opened new areas: The MPIE now has a Team Green which is committed to create a sustainable and ecological working environment. The health management revealed that the overall working conditions are above average and so is also the overall working satisfaction. Our MPIE gender equality plan was awarded "silver" by the Max Planck Society.

This report is structured into four parts:

— *Part I* contains information on recent scientific developments, new scientific groups, large network activities, new scientific laboratories, and on the work and life at the MPIE.
— *Parts II* and *III* cover the research activities of the institute. Part II provides a description of the scientific activities in the departments and Part III contains selected highlights, which summarize major recent scientific achievements in several topical areas of common interest.
— *Part IV* summarizes statistically relevant information about the institute.

The Directors of the MPIE

Düsseldorf, December 2021