

***Porous Metal Genomics for Tailoring Mechanical Properties of Light-weight 3D-Printed Architectures (PORMETALOMICS)***

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Porous metals, with pore diameters from nano to millimeters, are increasingly important in technology. Their high surface-to-volume ratio together with optimizable mechanical properties makes them promising candidates in various emerging applications such as metallic scaffolds for load-bearing bones, lightweight structures for transport technologies, electrodes for electrochemical energy storage devices and more. Additionally, 3D printing opens new horizons in additively manufactured complex porous architectures with desired properties. However, the enormous variety of possible morphologies makes it non-trivial to optimize the structure to tailor its mechanical properties. In order to fully harness the opportunities created by porous structures and to successfully incorporate them in next-generation devices, this project builds (a) fundamental understanding of the relation between the structure's morphology and the mechanical properties across the length-scales; (b) quantitative and exploitable structure-properties relationships, and (c) implement machine learning-based design in the vast morphological configuration space. These new capabilities are incorporated into state-of-the-art 3D printing, enabling the creation of tailor-designed structures with desired mechanical properties.

In the spirit of materials genomics, PORMETALOMICS project is focused on the development of methodology to characterize the morphology of porous structures. The resulting geometrical and topological descriptors are used to characterize many morphologies as well as to enumerate new structures with statistical importance, e.g. with unique topologies and/or geometries. Material modelling tools applied to the same dataset give their mechanical response to load, paving the way to direct relation between invariants and mechanical properties. The latter, captured within machine learning models, are employed to assess the mechanical property of various prototype structures of new morphologies via implementation of hierarchical screening, genetic algorithms or other machine learning techniques. Finally, an experimental 3D-printing effort is tightly integrated with the modelling part of the project with the goal of experimental verification of methodology, hyperparameter tuning, and execution and characterization of the identified important (e.g. best-performing) candidate structures.

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