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## **Semantic Materials Science**

Harnessing the Power of Semantic Web Technologies in Materials Science

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## **Preface**

Advanced technological solutions play a vital role in leveraging the potential of data and driving innovative research. However, the compatibility issues arising from different formats and structures of scientific data hinder progress in data generation, organization, storage, and sharing. To address these challenges, interoperability and efficient data access and analysis automation are crucial. The Semantic Web emerges as a powerful solution to overcome these obstacles.

Expanding and adapting Semantic Web technologies to the Materials Science domain can significantly enhance research outcomes by enabling the uniform consideration, integration, and analysis of heterogeneous data from diverse sources and formats. Implementing these technologies can improve the traceability and reproducibility of scientific procedures, experiments, and simulations. It also facilitates automatable data management solutions and empowers researchers to answer scientific inquiries using semantic queries. Moreover, machine learning methods can benefit from enhanced data completeness and coherence.

The primary objective of this workshop was to gather professionals in Semantic Web and in Materials Science and Engineering to show the recent advances in the use of Semantic Web technologies for Materials Science and Engineering, as well as provide a platform for discussing issues, finding collaboration opportunities and developing a community for this interdisciplinary field.

The contributions collected in this volume reflect the dynamic and diverse developments in the field of Semantic Materials Science. The proceedings open with the invited keynote by Roger H. French, who presented the Materials Data Science Ontology (MDS-Onto), a comprehensive approach for semantic data management in synchrotron science that combines FAIR principles, machine learning, and reasoning. The following contributions cover a broad spectrum of innovations: from the deep, ontology-based integration of manufacturing and simulation processes for fiber-reinforced materials (OntOMat) to the forward-looking use of LLM-driven multi-agent systems on semantically enriched knowledge graphs for inspection planning in non-destructive testing. Further contributions are dedicated to fundamental methodological challenges, such as the formal semantic representation of processes using Ontology Design Patterns, as well as pressing strategic goals, as outlined in the position paper on FAIR data management for the design of sustainable materials. The volume is concluded by a practical experience report, which illuminates the potentials and challenges of using LLMs and knowledge graphs for knowledge transfer in the traditional manufacturing industry.

We would like to express our sincere gratitude to all authors for their submissions, reflect current research in the field of semantic materials science. Furthermore, we would like to thank all members of the SeMatS program committee for their expertise and commitment to providing careful, constructive reviews and comments. Special thanks goes to our two keynote speakers, Roger H. French and Amila Akagić, for their inspiring presentations.

Finally, we extend our thanks to Blerina Spahiu and Juan Sequeda, the workshops chairs of the 24th International Semantic Web Conference (ISWC 2025), for their continuous support during the organization of the workshop.

November 2025

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