Big data in Materials Science –
Managing and exploiting the raw material of the 21st century

Symposium at the DPG Meeting 2018, Berlin, within the MM Division

Organizers

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and

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Materials science is entering an era where the growth of data from experiments and simulations is expanding beyond a level that is addressable by established scientific methods. The so-called "4 V challenge" – concerning Volume (the amount of data), Variety (the heterogeneity of form and meaning of data), Velocity (the rate at which data may change or new data arrive), and Veracity (uncertainty of quality) is clearly becoming eminent. Issues are, for example, an early discrimination between valuable and irrelevant experimental data, understanding errors in both experiment and theory, and assigning error bars and trust levels to density-functional theory high-throughput screening results, just to name a few.

Big Data of materials science, however, can also be seen as a chance, promising completely new insight and knowledge gain when fully exploiting the information content in the already available and strongly increasing data. This exploitation requires new and dedicated technology based on approaches in statistical and machine learning, compressed sensing, and other recent technologies from mathematics, computer science, statistics, and information technology. Making use of this synergy, will enable the development of novel, domain-specific, and even property-specific methods to enter and shape the era of data-driven materials research.

Invited speakers

Stefano Curtarolo, Duke University, USA *(Challenges of running large data collections in materials science)*

Manuel Guizar-Sicairos, Paul Scherrer Institut, Villigen, Switzerland *(Tensor tomography of anistropic and inhomogeneous materials)*

Cecile Hebert, EPFL Lausanne, Switzerland *(Data diagnostics in electron microscopy)*

Christoph Schweizer, Frauenhofer IWM, Germany *(Digital representation of materials and microstructure-property-relationships; ontology and metadata)*

Jilles Vreeken, MPI Saarbrücken, Germany *(Discovering Interpretable Patterns, Correlations, and Causality)*

Jan Vybíral, Czech Technical Univeristy, Prague, Czech Republic *(Compressed sensing for data analytics in materials science)*