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The MARVEL Initiative and the Integration of the Fifth Paradigm of Science

Dr. Pierre Villars

Material Phases Data System (MPDS), Vitznau, Switzerland

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Abstract: Confronted with the explosion of computing power, as well as materials data information Gray proposed in 2009 the Fourth Paradigm of Science: Data-Intensive Discovery through Data Exploration (eScience), which means to electronically unify experiment, theory and computation. The executive office of the president National Science and Technology Council of the United States has launched mid-2011 the whitepaper Materials Genome Initiative for Global Competitiveness having as major aim to shorten the time between discovery of advanced materials and its industrial application by at least a factor two. In 2014 JST has started a Japanese Project called Materials Informatics, Materials Design by Digital Data Driven Method. In the same year SNSF (Switzerland) has started the NCCR MARVEL Initiative called Material's Revolution: Computational Design and Discovery of Novel Materials.
Reflecting these new trends, many ideas have been proposed to explore new dimensions trying to derive interesting knowledge from a simple collection of many data. To show a clear direction for such trends, it is necessary to draw a roadmap by taking advantage of scientific data, namely in case of this publication we select scientific data on materials.

Neither the Fourth Paradigm of Science nor any of the above mentioned Initiatives can be realized without the extension to the Fifth Paradigm of Science: *Data-Intensive Discovery through Strategic Data Exploration by searching for Governing Factors with the aim to formulate Restraint Conditions*. This means data-intensive discovery through data exploration can only be realized if it is done in a strategic way and with a clear focus.

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The infinite high number of potential chemical element combination possibilities (equal to potential Novel Materials) forces us to develop approaches which are able to reduce this infinite number to a realistic number of most probable, to be calculated and experimentally investigated, potential Novel Materials.

The Fifth Paradigm has to be realized at the following levels: selection, discovery and design sciences with intention and focus converging to a solution heuristically. It is expected to be more strategic, dynamic, faster and holistic than above-mentioned initiatives, which are based on the Fourth Paradigm.
We outline how a trustworthy MARVEL can be strategically generated by high-throughput quantum simulations as well as CAPLHAD calculations to bridge the Fourth Paradigm and the Fifth Paradigm in case of materials science and engineering.

It is essential to notice that the realization of the Fourth and Fifth Paradigm requires three pre-conditions beforehand being established so as to control the above-mentioned heuristic processes properly:

i) *The first requirement is the introduction of the Prototype Classification.* This has to be done in a fully standardized way, so that the atom coordinates can be directly being compared, otherwise not even crystallographic databases done by different organizations can be linked. It is a pre-condition for the second requirement.

ii) *The Second requirement is the introduction of the Distinct Phases Concept being able to link different kind of materials databases* such as crystal structure, any intrinsic physical properties, and phase diagram information, etc., as well as databases produced by different expert teams. Otherwise it is impossible to link them by machine.

iii) *The third requirement is the existence of a fully standardized materials database concept (DBMS) to be used as reference database(s) system*. In addition the experimentally determined materials data have to be critically evaluated and cover the world literature comprehensively, as well as cover above specified different materials fields for single phase materials.

The above three outlined pre-conditions are worldwide only realized in the PAULING FILE project (http://www.paulingfile.com).

Keywords: Materials data exploration, PAULING FILE, eScience, materials design, materials discovery, MARVEL initiative, Materials Informatics initiative, Materials Genome initiative, Fourth Paradigm of science, Fifth Paradigm of science