MARVEL

THEOS
THEORY AND SIMULATION OF MATERIALS

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Accelerating Materials Design – Data Discovery versus Data Searching

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Abstract: Determining the key underlying *structure–property–functionality* relationships that control behavior within a *family of materials* reduces the data dimensionality required for accelerating materials design and discovery. Uncovering or discovering such relations in an ever-growing collection of heterogeneous data is often done by intuition, insight, or trial-and-error; yet they are mostly missed or masked within the data.

The competing issues are an increase in data complexity versus extraction of manageable representations to correlate properties. A goal then should be to develop techniques to extract predictive property relations that cannot be divined by intuition or extrapolated from existing models in competing classes of materials. From well-known examples, "data search" methods are shown not to have divined the underlying simple property-function relationships [1]. What is required are methods for *data discovery* [2]. Genetic programs (GPs) – genetic algorithms (GAs) that evolve computer programs similar to genetics and natural selection – are one method to regress symbolically key functional relations within data, i.e. "data discovery", and will be exemplified [3].

[1] Wang and Johnson, J. Amer. Chem. Soc. **131,** 14023-29 (2009).
[2] Zarkevich and Johnson, Phys. Rev. Lett. **113,** 265701 (2014).
[3] Zarkevich and Johnson, Phys. Rev. B **90,** (R)060201 (2014).
[4] Sun and Johnson, Phys. Rev. B **87,** 104107 (2013).
[5] Kibey et al., Acta Mater. **55,** 6843-6851 (2007), and Phys. Rev. B. **79,** 214202 (2009).