

Abstract Submitted
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Big Data of Materials Science – Critical Role of the Descriptor LUCA M. GHIRINGHELLI, Fritz-Haber-Institut der MPG, Berlin, DE, JAN VYBIRAL, Charles University, Prague, CZ, SERGEY V. LEVCHENKO, Fritz-Haber-Institut der MPG, Berlin, DE, CLAUDIA DRAXL, Humboldt-Universität zu Berlin, DE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Statistical learning of materials properties or functions so far starts with a largely silent, non-challenged step: the introduction of a multidimensional descriptor. However, when the scientific relationship of the descriptor to the actuating mechanisms is unclear, causality of the trained (learned) descriptor-property relation is uncertain. Thus, scientific advancement, trustful prediction of new promising materials and identification of anomalies is doubtful. We discuss and analyse this issue and define requirements for a descriptor that is suited for statistical learning of materials properties and functions. We show how a meaningful descriptor can be found systematically, by means of compressed sensing techniques. These concepts are demonstrated for examples in materials science: prediction of the relative stability of zincblende/wurtzite vs rocksalt octet binary semiconductors, and prediction of their band gaps, by using simple atomic input for building the descriptor.

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