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Finding descriptors for material properties from billions of candidates via compressed sensing: accurate prediction of crystal structures and band gaps from only chemical composition RUNHAI OUYANG, EMRE AHMETCIK, LUCA M. GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Identifying the key physical parameters (termed descriptor) determining the target material properties is a critical step toward material discovery and rational design. Thus far, systematic methods for the descriptor identification are not well established. In particular, it has been suggested that good descriptors should both yield an accurate prediction and be physically interpretable [L. M. Ghiringhelli,*et al.*, PRL **114**, 105503 (2015)]. In this talk, we present a systematic scheme for descriptor identification based on sure independent screening [J. Fan and J. Lv, J. R. Statist. Soc. B **70**, 849 (2008)] and compressed sensing [E. Cands and M. B. Wakin, IEEE Signal Proc. Mag. **25**, 21 (2008)]. The scheme starts with automatic building of the "feature spaces", i.e. all offered candidate descriptors, and the feature space may contain billions of options. The employed combination of sure independent screening and compressed sensing provides an efficient scheme for identifying the best low-dimensional descriptor. The approach is demonstrated for the important problems of crystal-structure and band-gap prediction.

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