

1st November 2017 - 2:00 p.m. CFEL-bldg. 99, seminar rooms I-II

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SISSO: a compressed-sensing method for systematically identifying physical models of materials properties

The lack of reliable methods for identifying descriptors – the set of parameters capturing the underlying mechanism of a materials property – is one of the factors hindering efficient materials development. SISSO (sure independence screening and sparsifying operator) tackles immense and correlated feature spaces (many billions of physical model candidates), and converges to the optimal solution from a combination of features relevant to the materials property of interest.

The methodology is applied to the showcase example of predicting the metal-insulator classification and to 2D quantum spin-Hall (topological) insulators (QSHI). The chemical bounding effect in the topological transitions appears naturally in the found model. We also suggest a new family of 74 QSHI candidates.



Host: Robin Santra – CFEL-DESY Theory Division